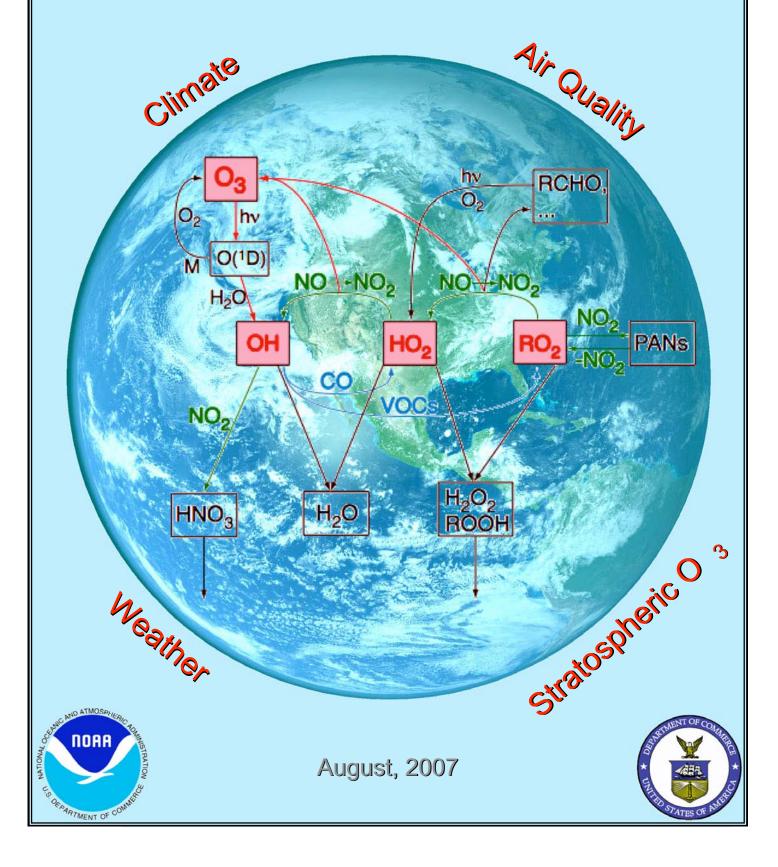
Atmospheric Chemistry Modeling

An Inventory of Model Platforms in use at NOAA



Contents

Introduction	3
Summary of NOAA Atmospheric Chemical Models	5
Global Models with Chemistry	-
Atmospheric Model with Transport and Chemistry (AMTRAC)	
AM3	
Flow-following finite-volume Icosahedral Model (FIM)	
Global Forecast System (GFS)	
Model for OZone And Related chemical Tracers (MOZART)	
Real-time Air Quality Modeling System (RAQMS)	
2-D Middle Atmosphere Model (NOCAR)	
Transport Models for Chemical Tracers	
Transport Model 5 (TM5) / Carbon Tracker	
FLEXPART	
Stochastic Time-Inverted Lagrangian Transport (STILT)	
Hybrid Single Particle Lagrangian Integrated Trajectory (HYSPLIT)	
Global Chemical Transport Model – Dust and Dissolved Iron (GCTM-Dust)	
Rapid Update Cycle / Colorado State University Lagrangian Particle Dispersion	
Model (RUC/CSU-LPDM)	
Infusing satellite Data into Environmental Applications (IDEA)	37
Regional Models with Chemistry	30
Community Multiscale Air Quality (CMAQ) Modeling System	
Weather Research and Forecasting / Chemistry Model (WRF/Chem)	
weather Research and Porceasting / Chemistry Woder (WRI / Chem)	
Local Scale Chemical Models	45
Cloud Parcel	47
Regional Atmospheric Modeling System in Large Eddy Simulation mode	
(RAMS/LES)	49
Master Chemical Mechanism (MCM) – Box Model	51
Model of Aerosols and Ions in the Atmosphere (MAIA)	53
Appendix A: NOAA Atmospheric Chemical Modeling Contact List	55

Introduction

Atmospheric chemical models are used throughout NOAA to better understand the complex chemical and physical interactions that determine atmospheric composition and characteristics on local to global scales. These models are also used to forecast the state of the atmosphere days to centuries into the future. This report provides an inventory of atmospheric chemical modeling platforms currently in use across NOAA. Most of the models described in this report were developed, and are sustained, through a broad, often international, collaboration involving scientists from the public and private sectors.

Model Applications:

NOAA applies atmospheric chemical models in a number of very diverse applications. Some of the modeling platforms are used in research applications to aid in the interpretation of atmospheric or laboratory measurements. Some are used in environmental assessments to evaluate impacts of policy and regulatory options. Some are used in an operational environment to forecast the distribution of atmospheric pollution. Current applications include the following:

<u>Climate</u> – Numerical models of climate are used to advance our understanding of the Earth's climate system and to generate products relevant to assessment and policy decision support. Specifically, these coupled chemistry-climate models:

- identify and elucidate the physical and dynamical mechanisms that maintain climate and cause its variations on seasonal to centennial time scales;
- assess understanding of the predictability of the climate system on seasonal and longer time scales, including the El Niño phenomenon; and
- evaluate the impact of human activity on the Earth's climate system.

The simulations and projections of NOAA's models are used in international climate assessments, most prominently those of the Intergovernmental Panel on Climate Change.

<u>Air Quality</u> – Predictive air quality models have three broad applications in air quality:

- Regulatory Analysis Air quality models are used to evaluate the relative benefits of emission management options to improve air quality. Regional air quality models and Lagrangian trajectory models are also used retrospectively to determine the sources that contribute to air pollution episodes.
- Forecasting NOAA has an operational air quality forecasting capability that currently provides daily surface ozone forecasts for the eastern U.S. and smoke forecasts for the lower 48 states (CONUS). The NWS plans to extend that capability to include the entire U.S. and is testing an experimental capability for ozone forecasts over the CONUS. A particulate matter (PM) forecast capability is in development.
- Research A wide variety of model types (box models, regional air quality models, trajectory models, etc.) are used in NOAA research programs aimed at a better understanding of atmospheric processes that influence air quality.

<u>Stratospheric Ozone</u> – Coupled chemistry-climate models are used to probe the dynamics, radiation, and chemistry of the stratosphere, especially with regard to the ozone layer. Both two-dimensional (2-D) and three-dimensional (3-D) models study multiple factors, such as solar influences and trace gas influences, to generate projections of both the climate and ozone effects. 3-D models are particularly useful in examining climate couplings and feedbacks. The 2-D models are used to calculate trace gas lifetimes, which are used in calculations of the global warming potentials of the gases. Simplified box models are applied to generate scenarios of future stratospheric chlorine and bromine emissions under various potential decision frameworks. All of these NOAA models have provided useful input to the international assessments of stratospheric ozone done periodically for the UNEP/WMO Montreal Protocol and its subsequent agreements that protects the stratospheric ozone layer.

<u>Weather</u> – Physical meteorology directly effects the emission, transport, mixing, transformation and removal of atmospheric pollutants. The presence of these contaminants can also modify the physical state of the atmosphere and hence impact the weather. The thermal structure of the atmosphere may be modified by the absorption of radiation by gaseous constituents and the absorption and scattering of radiation by particles. In addition, particles can affect cloud microphysics and impact the physical and optical properties of clouds. Thus, state-of-the-art weather forecast models now strive to simulate the chemical state of the atmosphere as well as the physical state in an effort to improve forecast accuracy by accounting for constituent effects on radiation, thermal structure, and cloud microphysics.

Model Types:

Each of the model platforms described in this report was developed with a specific application in mind. The diverse set of applications results in an equally diverse collection of model architectures including the manner in which the various models represent chemical processes and transport. For example, the inventory includes a box model that is used to evaluate chemical mechanisms through an extremely detailed representation of gas-phase atmospheric chemistry and no treatment of transport. At the other extreme are global transport models that provide a detailed representation of pollutant transport in three dimensions without any provision for chemical transformation. The models in the inventory have been grouped in the following categories to facilitate the

review of this diverse set of models. Several of the models could have been placed in multiple categories. In these cases the models have been placed in the category that best describes their primary functionality.

<u>Global Models with Chemistry</u> – This category includes model platforms that are designed to operate on a global scale and include the capability to simulate atmospheric chemical transformations on this scale. These models may be designed specifically for only a part of the atmosphere (e.g., the stratosphere) with only a rudimentary treatment of the remainder of the atmosphere.

<u>Transport Models for Chemical Tracers</u> – These models are used either retrospectively to determine the history of specific air masses or prospectively to forecast the fate of these air masses. These models are typically used to track relatively inert pollutants (e.g., CO₂, dust, CO, etc.) as they move from source to receptor regions.

<u>Regional Models with Chemistry</u> – This group includes the regional air quality models, which are typically, but not exclusively, Eulerian models that run on scales from hundreds to thousands of kilometers.

<u>Local Scale Chemical Models</u> – This category includes a very diverse set of models that are used primarily for applications on a local scale related to a specific aspect of atmospheric dynamics and/or chemistry (e.g., cloud microphysics, detailed gasphase or heterogeneous chemistry, aerosol formation and growth, etc.).

NOAA Atmospheric Chemical Model Summary

Model Name	Рабе	Lab	Technical	Forecast	Trono	Strat	Global	Reg	Local	Trans Ch	Aerosol Chem C	osol	Output
AM3		GFDL	L. Horowitz		-	>	>	>		>	7		Online global trop & strat chem, chemistry-
AMTRAC	6	GFDL	J. Austin		>	>	>			7	7		Strat O ₃ depletion & recovery, climate change impact on strat chem
Cloud Parcel	47	ESRL	B. Ervens		>				~	>	>	>	Cloud chemistry and microphysics
СМАО	41	ARL	R. Mathur	>	>			>	>	>	7	>	Regional forecast guidance and assessments for O ₃ , PM, & air toxic distributions
FIM	13	ESRL	S. Benjamin	>	>		>			7	~		Global tracer & chem model, under development
FLEXPART	27	ESRL	O. Cooper	>	>	>	>	>		>			Global/regional pollutant transport, source attribution, field mission support
GCTM-Dust	33	GFDL	SM. Fan		>		>			>	7		Global dust transport, acidification, dissolved iron denosition
GFS	15	NCEP	S. Lu	>	>	>	>			>		>	Medium-range weather prediction/ research,
TIVEBLU	1,0	A D.I.	0 G	,	-		,	-	-				boundary conditions for other models
HISPLII	31	AKL	K. Draxier	>	>		>	>	>	>			Follutant transport, dispersion, deposition, forecasting
IDEA	37	NESDIS	S. Kondragunta	>	>			>		>	>		PM satellite data assimilation, regional PM
MAIA	53	ESRL	J. Kazil E. R. Loveiov	>	>	>			>	~	>	>	Aerosol formation and growth
MCM Box	51	ESRL	R. Sommariva		>				>	>	>		Chem mechanism development, plume chem
MOZART	17	ESRL/ GFDL	C. Granier		>		>			>	7		Evolution of global chem distributions, observational analysis. assessments
NOCAR	21	ESRL	R. Portmann S. Solomon			>	>			>	7		Strat O ₃ evolution and depletion potentials, source gas lifetimes
RAMS/ LES	49	ESRL	G. Feingold		>				>	>	>	>	Aerosol-cloud interactions
RAQMS	19	NESDIS	R. B. Pierce	>	>	>	>			7			Global chem satellite data assimilation & analysis, field mission support
RUC/ CSU-LPDM	35	ESRL	S. Benjamin	>	>			>		>			Rapid update weather prediction, tracer transport, pollutant source attribution
STILT	56	ESRL	A. Hirsch	>	>			>		>			Greenhouse gas transport and source analysis
TM5			W. Peters/	>	>		>			7	7		Global/regional chem tracer transport, pollutant
Carbon Tracker	25	ESRL	A. Jacobson	-				-		-			source & sink analysis
WRF/Chem	43	ESRL	G. Grell	>	>		>	>	>	>	7		Regional online forecasting & analysis of O_3 & PM, climate-AQ interactions

See explanation of column titles on next page.

Explanation of Column Headings:

Lab NOAA Laboratory primarily responsible for model development

Technical

Contact Principal contact person(s) for model (see detailed reports for complete list of model participants and their contact information)

Forecast Model makes regular forecasts of atmospheric chemical transport and/or transformations

Trop Model has explicit treatment of tropospheric chemistry and/or transport

Strat Model has explicit treatment of stratospheric chemistry and/or transport

Global Model can treat global scale chemistry and/or transport

Reg Model can treat regional scale chemistry and/or transport

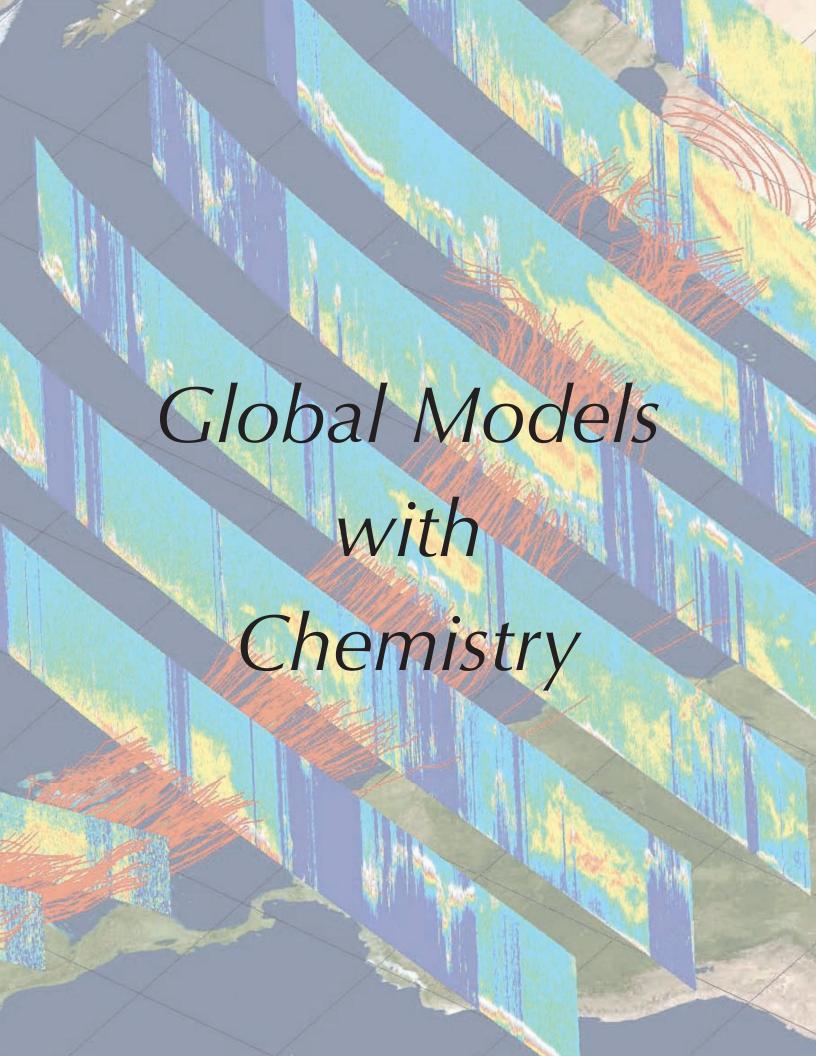
Local Model can treat local scale (domain ~100 km x 100 km or smaller) chemistry and/or transport

Trans Model explicitly calculates transport of chemical species

Chem Model has explicit treatment of gas phase chemical reactions

Aerosol Model has explicit treatment of aerosol transport, chemical reactions, and/or microphysics

Cloud Model has explicit treatment of cloud droplet transport, chemical reactions, and/or microphysics



Atmospheric Model with Transport and Chemistry (AMTRAC)

1. Brief description of model

Climate model with coupled stratospheric chemistry and simplified tropospheric chemistry.

2. Principal applications or customers

Timing and extent of ozone depletion and recovery.

Impact of climate change on stratospheric chemistry.

3. Key participants, lab/organization, effort, contact information

John Austin, UCAR/GFDL (full time).

John Wilson, GFDL (part time).

4. Literature citations, reports, or websites with detailed model description

Austin and Wilson, J. Geophys. Res., 111, D16314, 2006.

5. Specifications

Domain: Global.

Horizontal resolution and grid/coordinate system: Grid Point uniform lat.-long. 2 deg. x 2.5 deg.

Vertical resolution and grid/coordinate system: 48 levels from the surface to 0.002 hPa (ca. 87 km), resolution decreasing at higher levels, about 2 km in the stratosphere.

Dynamical and numerical transport schemes: Finite volume.

Chemistry and aerosol schemes: Euler backward sparse matrix inversion for chemistry, aerosol surface areas deduced from optical depths.

Planetary boundary layer and land-surface schemes: As in underlying climate model AM2 (Anderson et al., *J. Clim., 17*, 4641-4673, 2004).

Deposition schemes: As in underlying climate model AM2 (Anderson et al., 2004).

Sub-grid parameterizations: As in underlying climate model AM2 (Anderson et al., 2004), Non-orographic gravity wave forcing scheme included (Alexander and Dunkerton, *J. Atmos. Sci., 56*, 4167-4182, 1999).

6. Sources of required data

Meteorological drivers/boundary conditions: Specified SSTs/sea ice from observations or models, solar fluxes at the top of the atmosphere.

Chemical boundary conditions/assimilations: Evolution of tropospheric CFCs, concentrations of the well-mixed GHGs.

7. Computational requirements

Hardware/software: SGI cluster with 30 intel processors, FORTRAN90.

Simulation time: 14 hours per model simulated year.

- 8. Description of key outcomes, applications (including literature citations describing work), and other information about modeling capabilities
 - (a) Decline and recovery of stratospheric ozone. Austin and Wilson (2006) showed that recovery of ozone was likely to be delayed about 15 years in the Antarctic relative to that previously expected, because of the additional time needed for halogen amounts to decline to 1980 levels. Ozone recovery in the Arctic was simulated to be earlier because of the increased strength of the circulation due to climate change. These results contributed to the 2006 WMO/UNEP assessment of ozone.
 - (b) Austin et al., *J. Atmos. Sci.*, 64, 905-921, 2007 showed that during certain periods in the last few decades stratospheric water vapor may have increased faster than anticipated on the basis of the methane increase alone. In model simulations this was caused by increased atmospheric circulation transport more methane in to the stratosphere and subsequent oxidation of the methane
 - (c) Eyring et al., J. Geophys. Res., 111, D22308, 2006 compared results from a range of different coupled chemistry climate

- models of the recent past. This showed agreement for many parameters, but also showed that several chemical species were very different in the individual models. These results contributed to the 2006 WMO/UNEP assessment of ozone.
- (d) The strength of the Brewer-Dobson circulation. Li et al., *J. Clim, accepted*, 2007 and Austin, J., and F. Li, *Geophys. Res. Lett.*, *33*, L17807, 2006 showed that the strength of the Brewer-Dobson circulation increased in the future, leading to the stratospheric air becoming younger (i.e., taking less time to transport from the troposphere).
- (e) The solar cycle in ozone and temperature. Austin, J., L.L. Hood, and B.E. Soukharev, *Atmos. Chem. Phys., in press*, 2007 showed AMTRAC simulations of the solar cycle in ozone and temperature and compared the results with measurements. This demonstrated better agreement with ozone measurements in the tropical lower stratosphere than had previously been achieved.

AM₃

1. Brief description of model

AM3 is a general circulation model (GCM) being developed at GFDL. It includes online, interactive tropospheric and stratospheric gas-phase and aerosol chemistry.

2. Principal applications or customers

Simulating global- and regional-scale climate and distributions of chemical species.

3. Key participants, lab/organization, effort, contact information

Larry W. Horowitz, GFDL, larry.horowitz@noaa.gov.

Paul Ginoux, GFDL, paul.ginoux@noaa.gov.

John Austin, GFDL/UCAR, john.austin@noaa.gov.

John Wilson, GFDL, john.wilson@noaa.gov.

Yi Ming, GFDL/UCAR, yi.ming@noaa.gov.

4. Literature citations, reports, or websites with detailed model description

AM2: GFDL Global Atmospheric Model Development Team (GAMDT): The new Geophysical Fluid Dynamics Laboratory (GFDL) global atmosphere and land model AM2/LM2: Evaluation with prescribed SST simulations, *J. Clim.*, 17(24), 4641-4673, 2004.

MOZART tropospheric chemistry: Horowitz, L., et al., A global simulation of tropospheric ozone and related tracers: Description and evaluation of MOZART, version 2, *J. Geophys. Res.*, 108(D24), 4784, doi:10.1029/2002JD002853, 2003.

AMTRAC stratospheric chemistry: Austin, J., and R.J. Wilson, Ensemble simulations of the decline and recovery of stratospheric ozone, *J. Geophys. Res.*, 111, D16314, doi:10.1029/2005JD006907, 2006; Austin, J., et al., Evolution of water vapor concentrations and stratospheric age of air in coupled chemistry-climate model simulations, *J. Atmos. Sci.*, 64(3), 905-921, 2007.

GOCART aerosols: Ginoux, P., et al., Sources and distributions of dust aerosols simulated with the GOCART model, *J. Geophys. Res.*, 106(D17), 20,255-20,273, 2001; Chin, M., et al., Tropospheric aerosol optical thickness from the GOCART model and comparisons with satellite and Sun photometer measurements, *J. Atmos. Sci.*, 59(3), 461-483, 2002.

Aerosol-cloud interactions: Ming, Y., et al., Modeling the interactions between aerosols and liquid water clouds with a self-consistent cloud scheme in a general circulation model, *J. Atmos. Sci.*, 64(4), 1189-1209, 2007.

5. Specifications

Domain: Global.

Horizontal resolution and grid/coordinate system: Various. Typically run at M45 (2° latitude x 2.5° longitude).

Vertical resolution and grid/coordinate system: Various. Typically 24 levels (L24, up to 4 hPa) for tropospheric version and 48 levels (L48, up to 0.3 hPa) for stratospheric version.

Dynamical and numerical transport schemes: Finite volume dynamical core [Lin, S.-J., Mon. Wea. Rev., 2004].

Chemistry and aerosol schemes: Tropospheric chemistry scheme and solver based on that in MOZART-2 [Horowitz et al., 2003], stratospheric chemistry based on that in UMETRAC [Austin and Butchart, 2003]. Chemistry is solved using an implicit backward Euler method with Newton-Raphson iteration. The solver is easily adaptable such that the species and reactions can easily be modified.

Planetary boundary layer and land-surface schemes: Lock et al. (2000) PBL scheme; interactive land surface model (LM3).

Deposition schemes: Dry deposition velocities calculated using a Wesely [1989]-type scheme. Wet deposition from large-scale and convective precipitation calculated using Giorgi and Chameides [1985] parameterization.

Sub-grid parameterizations: Donner [1993] deep convection scheme, Bretherton et al. [2004] shallow convection.

Sources of required data

Meteorological drivers/boundary conditions: Can be nudged to reanalyses (e.g., NCEP or ECMWF).

Chemical boundary conditions/assimilations: TES O₃ data has been assimilated into AM2-CHEM by D. Jones et al. (U. Toronto).

Emission inventories and temporal/spatial processing: Various. "Standard" emissions are: monthly mean emissions of gases from

EDGAR-2 (as in MOZART-2 [Horowitz et al., 2003]); aerosol emissions compiled for AEROCOM [Dentener et al., Atmos. Chem. Phys., 2006].

7. Computational requirements

- Hardware/software: Can be run on a variety of platforms. At GFDL, AM3 is run on an SGI Altix multiprocessor system.
- Simulation time: Varies with model resolution, amount of chemistry included in the simulation, and number of processors used. On 60 Altix processors at M45L24 resolution, model takes ~15 minutes for physical model, and 45-60 minutes for full-chemistry model.
- 8. Description of key outcomes, applications (including literature citations describing work), and other information about modeling capabilities

Additional Detailed Model Description:

AM3 is a general circulation model (GCM) being developed at GFDL. It includes online, interactive tropospheric and stratospheric gas-phase and aerosol chemistry. The AM3 GCM includes improvements to moist physics and aerosol-clouds interactions from an earlier version of the model, AM2 [GFDL GAMDT, 2004]. The tropospheric emissions, chemistry, and deposition schemes are based on those in the MOZART-2 [Horowitz et al., 2003; Tie et al., 2005] and GOCART [Chin et al., 2000, 2002; Ginoux et al., 2001] chemical transport models. Stratospheric chemistry is from UMETRAC [Austin and Butchart, 2003], and has previously been incorporated into the AMTRAC model based on AM2. The current version of AM3 includes tropospheric ozone-NO_x-CO-hydrocarbon and aerosol (sulfate, nitrate, ammonium, carbonaceous, dust, and sea salt) chemistry and stratospheric chemistry, including a total of ~100 chemical species and ~200 chemical and photochemical reactions. The chemical solver in AM3 is flexible such that the species and reactions included can easily be modified.

a. Stratospheric studies (AM2/AMTRAC)

- Austin, J., J. Wilson, F. Li, and H. Vömel, Evolution of water vapor concentrations and stratospheric age of air in coupled chemistry-climate model simulations, *J. Atmos. Sci.*, 64(3), 905-921, 2007.
- Austin, J., L.L. Hood, and B.E. Soukharev, Solar cycle variations of stratospheric ozone and temperature in simulations of a coupled chemistry-climate model, *Atmos. Chem. Phys.*, 7, 1693-1706, 2007.
- Austin, J., and R.J. Wilson, Ensemble simulations of the decline and recovery of stratospheric ozone, *J. Geophys. Res.*, 111, D16314, doi:10.1029/2005JD006907, 2006.

b. Offline ozone and aerosol distributions (MOZART/AM2)

- Ginoux, P., L.W. Horowitz, V. Ramaswamy, I.V. Geogdzhayev, B.N. Holben, G. Stenchikov, and X. Tie, Evaluation of aerosol distribution and optical depth in the Geophysical Fluid Dynamics Laboratory coupled model CM2.1 for present climate, *J. Geophys. Res.*, 111, D22210, doi:10.1029/2005JD006707, 2006.
- Horowitz, L.W., Past, present, and future concentrations of tropospheric ozone and aerosols: Methodology, ozone evaluation, and sensitivity to aerosol wet removal, *J. Geophys. Res.*, 111, D22211, doi:10.1029/2005JD006937, 2006.
- Ming, Y., V. Ramaswamy, P.A. Ginoux, and L.W. Horowitz, Direct radiative forcing of anthropogenic organic aerosol, *J. Geophys. Res.*, 110, D20208, doi:10.1029/2004JD005573, 2005.

c. Aerosol indirect effect

- Ming, Y., V. Ramaswamy, L.J. Donner, V.T.J. Phillips, S.A. Klein, P.A. Ginoux, and L.W. Horowitz, Modeling the interactions between aerosols and liquid water clouds with a self-consistent cloud scheme in a general circulation model, *J. Atmos. Sci.*, 64(4), 1189-1209, 2007.
- Ming, Y., V. Ramaswamy, L.J. Donner, and V.T.J. Phillips, A new parameterization of cloud droplet activation applicable to general circulation models, *J. Atmos. Sci.*, 63(4), 1348-1356, 2006.
- Ming, Y., V. Ramaswamy, P.A. Ginoux, L.W. Horowitz, and L.M. Russell, Geophysical Fluid Dynamics Laboratory general circulation model investigation of the indirect radiative effects of anthropogenic sulfate aerosol, *J. Geophys. Res., 110*, D22206, doi:10.1029/2005JD006161, 2005.

Flow-following finite-volume Icosahedral Model (FIM)

1. Brief description of model

Global 3-D dynamic model under development at ESRL. Uses icosahedral horizontal grid to avoid pole problem, uses finite-volume horizontal advection and isentropic-sigma vertical coordinate, both of which provide improved conservation and accuracy for tracer advection. Currently using only GFS precip/radiation/boundary-layer/land-surface physics, suitable for chemistry in future (e.g., WRF/Chem schemes).

2. Principal applications or customers

Alternative global model for NCEP global ensemble, possible flagship model for ESRL research using ESRL coupled assimilation-modeling on global scale.

3. Key participants, lab/organization, effort, contact information

Jin Lee, Rainer Bleck, Jian-wen Bao, Stan Benjamin, John Brown, and Jacques Middlecoff, ESRL GSD/PSD.

Primary contact – Jin Lee, Stan Benjamin.

4. Literature citations, reports, or websites with detailed model description

http://fim.noaa.gov/fimdocu rb.pdf.

5. Specifications

Domain: Global.

Horizontal resolution and grid/coordinate system: Variable resolution, Horizontal-icosahedral, current testing at 240-30 km horizontal.

Vertical resolution and grid/coordinate system: Variable resolution, isentropic-sigma, current testing at 50 levels vertical.

Dynamical and numerical transport schemes: Finite-volume, flux-corrected transport.

Chemistry and aerosol schemes: None yet, future adaptation of WRF/Chem schemes in future.

Planetary boundary layer and land-surface schemes: GFS PBL, GFS-Noah Land-surface currently, possibly will change to WRF components in future.

Deposition schemes: None currently.

Sub-grid parameterizations: GFS simplified Arakawa-Schubert scheme.

6. Sources of required data

Meteorological drivers/boundary conditions: GFS data, reanalysis data.

Chemical boundary conditions/assimilations: None yet, planned to be linked with NCEP GSI assimilation code (global configuration).

Emission inventories and temporal/spatial processing: None at this time.

7. Computational requirements

Hardware/software: Runs on multiple-processors allotments on ijet/wjet/ejet.

8. Description of key outcomes, applications (including literature citations describing work), and other information about modeling capabilities

None listed.

Global Forecast System (GFS)

1. Brief description of model

Global spectral model for medium-range weather predictions and atmospheric research.

2. Principal applications or customers

Weather forecasts out to 16 days.

Forecasts routinely used by NWS field offices, other government agencies, the private sector, and the public.

3. Key participants, lab/organization, effort, contact information

Sarah Lu, NOAA/NCEP/EMC, full-time, sarah.lu@noaa.gov.

Ho-Chun Huang, NOAA/NCEP/EMC, full-time, ho-chun.huang@noaa.gov.

4. Literature citations, reports, or websites with detailed model description

Moorthi et al., Changes to the 2001 NCEP Operational MRF/AVN Global Analysis/Forecast System, NOAA Technical Bulletin No. 484, available at NOAA/NWS/NCEP, Camp Springs, Maryland, 2001.

Global Climate & Weather Modeling Branch, 2003, The GFS Atmospheric Model, NCEP Office Note 442, available at http://www.emc.ncep.noaa.gov/officenotes.

5. Specifications

Domain: Global

Horizontal resolution and grid/coordinate system: Spectral triangular 382 (approximately 35 km resolution).

Vertical resolution and grid/coordinate system: Hybrid sigma-pressure coordinate, 64 layers from surface to ~ 0.2 mb.

Dynamical and numerical transport schemes: Leapfrog for nonlinear advection; semi-implicit for gravity wave and zonal advection of moisture and vorticity.

Chemistry and aerosol schemes: Ozone: Naval Research Lab (NRL) ozone physics algorithm (production and destruction are parameterized from monthly and zonal mean dataset derived from NRL 2-D ozone chemistry model);

Aerosols: NASA GOCART (planned activities).

Planetary boundary layer and land-surface schemes: PBL: Non-local boundary layer diffusion scheme of Hong and Pan (1996); Land-surface: Noah.

Deposition schemes: NA

Sub-grid parameterizations: Simplified Arakawa-Schubert scheme for convective cumulus parameterization.

6. Sources of required data

Meteorological drivers/boundary conditions: NA

Chemical boundary conditions/assimilations: SBUV/2 assimilation for stratospheric ozone (above 250 mb).

Emission inventories and temporal/spatial processing: NA

7. Computational requirements

Hardware/software: NCEP CCS machine; FORTRAN90.

Simulation time: 66 minute wall-clock time for 7.5 days T382L64 simulation using 13 nodes (32 logical CPUs per node).

- 8. Description of key outcomes, applications (including literature citations describing work), and other information about modeling capabilities
 - a. Operational medium-range weather forecasts: GFS provides weather forecasts up to 384 hours at 00, 06, 12, and 18 UTC cycles over global domain. Products in digital and graphic formats are available at AWIPS, NWS MOS website, and NCEP Model Analysis and Forecast website.
 - b. Lateral boundary conditions for WRF: GFS forecasts provide meteorological lateral conditions for WRF.
 - c Lateral boundary conditions for CMAQ-WRF: GFS ozone analyses provide ozone lateral conditions for CMAQ-WRF.
 - d. Planned activities: NCEP EMC is developing aerosol forecasting capability in GFS based on NASA GOCART. Both offline

approach (using GFS output to drive GOCART) and in-line approach (couple GFS and GOCART using ESMF coupler) are in progress. CMAQ-WRF regional air quality lateral and top boundaries and initial aerosol conditions will be specified from GFS-GOCART for testing and possible operational implementation.

Model for OZone And Related chemical Tracers (MOZART)

1. Brief description of mode

MOZART is a global chemical transport model, driven with offline meteorology (e.g., from NCEP or ECMWF reanalyses, or from a GCM).

Principal applications or customer

Studies of the evolution of the global distribution of chemical species (gases and aerosols) for present, past (1860-2000), and future (2000-2100) periods. Analysis of observation campaigns. Analysis of satellite data and inverse modeling. Participation in international assessments.

Key participants, lab/organization, effort, contact information

NOAA: Claire Granier (claire.granier@noaa.gov), ESRL/CSD; Larry Horowitz (larry.horowitz@noaa.gov); Arlene Fiore (arlene.fiore@noaa.gov), GFDL.

NCAR: L. Emmons (emmons@ucar.edu), P. Hess, J.-F. Lamarque, D. Kinnison, J. Orlando, G. Pfister, X. Tie, G. Tyndall, S. Walters. FZ Juelich, Germany: M. Schultz (m.schultz@fz-juelich.de), O. Stein.

4. Literature citations, reports, or websites with detailed model description

Emmons, L.K., et al., Sensitivity of chemical budgets to meteorology in MOZART-4, *EOS Trans. AGU, 87*(52), Fall Meet. Suppl., Abstract A51C-0094, 2006.

Horowitz, L., et al., A global simulation of tropospheric ozone and related tracers: Description and evaluation of MOZART, version 2, *J. Geophys. Res.*, 108(D24), 4784, doi:10.1029/2002JD002853, 2003.

Kinnison, D.E., et al., Sensitivity of chemical tracers to meteorological parameters in the MOZART-3 chemical transport model, *J. Geophys. Res., in press*, 2007.

Tie, X., et al., Assessment of the global impact of aerosols on tropospheric oxidants, *J. Geophys. Res.*, 110, D03204, doi:10.1029/2004JD005359, 2005.

http://www.gctm.acd.ucar.edu/mozart/.

http://www.gfdl.noaa.gov/~lwh/mozart/mozart.html.

5. Specifications

Domain: Global.

Horizontal resolution and grid/coordinate system: Variable, adjustable to the meteorology data.

Vertical resolution and grid/coordinate system: Variable, adjustable to the meteorology data (e.g., 1.9 x 1.9 degrees, 28 vertical levels for use with NCEP reanalysis).

Dynamical and numerical transport schemes: Advection: Lin and Rood (1996); Convection: Zhang and McFarlane (1995), Hack (1994); Boundary layer: Holtslag and Boville (1993).

Chemistry and aerosol schemes: Variable. MOZART-4 contains 98 chemical species and about 200 chemical reactions; O₃, CO, NO_y compounds, HO_x compounds, several hydrocarbons and their oxidation compounds, SO₂, SO₄⁻, H₂SO₄, black carbon, organic carbon, SOA, DMS, about 200 chemical reactions.

Planetary boundary layer and land-surface schemes: PBL parameterization: Holtslag and Boville (1993).

Deposition schemes: Based on the approach of Wesely (1989); MOZART-4 includes an interactive deposition scheme.

Sub-grid parameterizations: Convection: Zhang and McFarlane (1995), Hack (1994); Boundary layer: Holtslag and Boville (1993).

6. Sources of required data

Meteorological drivers/boundary conditions: NCEP, ECMWF, or archives from global circulation models.

Chemical boundary conditions/assimilations: MOZART has been used for assimilation/inverse modeling of GMD CO surface observations and for MOPITT and TES satellite observations.

Emission inventories and temporal/spatial processing: Variable. Standard emissions for MOZART-4: POET database (*Granier et al.*, 2005), available from: http://www.aero.jussieu.fr/projet/ACCENT/POET.php. Other emissions used: RETRO database, EDGAR database and the GICC database under development. Biomass burning emissions for specific years are available from GFED (Global Fire Emissions Database). Biogenic emissions of hydrocarbons and NO_x are calculated interactively.

7. Computational requirements

Hardware/software: MOZART tested on computing platforms ranging from a single CPU on a desktop machine to more than one hun-

dred CPUs on a state-of-the-art supercomputer. MOZART uses MPI and/or OpenMP parallelization, depending on the platform.

Simulation time: Depends on the platform. On the current IBM clustered Symmetric Multi Processing system at NCAR or the SGI Altix system at GFDL, one day of simulation takes less than 5 minutes for simulations at T42 (2.8 x 2.8 degrees) or T62 (1.9 x 1.9 degrees) resolution.

 Description of key outcomes, applications (including literature citations describing work), and other information about modeling capabilities

Model Description:

The most recent tropospheric version, MOZART-4 [*Emmons et al.*, in preparation], includes a number of improvements over MOZART-2 [*Horowitz et al.*, 2003]. The chemical mechanism includes an updated isoprene oxidation scheme [*Tyndall et al.*, 2001] and a more detailed treatment of higher volatile organic compounds (VOCs), including: a "bigalk" (C_5H_{12}) tracer, a lumped species representing the butanes, pentanes, and hexanes; "bigene" (C_4H_8), a lumped species representing mostly 2-methyl-propene and 2-butene; "toluene" (C_7H_8), a lumped aromatic compound representing mostly benzene, toluene, and the xylenes. Other model improvements include online calculation of dry deposition, online calculation of biogenic isoprene and monoterpenes and soil NO emissions, and the online photolysis scheme, FTUV (fast-TUV), based on the TUV (Tropospheric Ultraviolet-Visible) model [*Tie et al.*, 2003]. The representation of aerosols in MOZART has been extended from the work by *Tie et al.* [2001, 2005], and includes the calculation of black carbon (hydrophobic and hydrophilic), primary organic (hydrophobic and hydrophilic), secondary organic, ammonium, nitrate, and sulfate aerosols. The uptake of N_2O_5 , HO_2 , NO_2 , and HO_3 on aerosols is included [*Jacob*, 2000]. There is also a version of MOZART which considers stratospheric chemistry, called MOZART-3 [*Kinnison et al.*, 2007].

MOZART is a model widely used in the international scientific community. It is currently used by several groups in the U.S., Europe, Brazil, China, and Japan. Routines from the MOZART-3 and MOZART-4 models are currently being introduced in the CCSM framework, under the CAM-CHEM coupled chemistry-climate modeling system, and in the GFDL AM3 GCM. MOZART is one of the 3 chemistry-transport models used by the European Center ECMWF in the ongoing GEMS system for forecasting the distribution of chemical species at different scales (details at http://www.ecmwf.int/research/EU_projects/GEMS/).

Effects of ship emissions:

Granier, C., et al., Geophys. Res. Lett., 33, L13807, doi:10.1029/2006GL026180, 2006.

Effects of aerosols on tropospheric chemistry:

Tie, X., et al., J. Geophys. Res., 106, 2931-2964, 2001.

Tie, X., et al., J. Geophys. Res., 108, 4642, doi: 10.1029/2003JD003659, 2003.

Tie, X., et al., J. Geophys. Res., 110, D03204, doi:10.1029/2004JD005359, 2005.

Radiative forcing and health impacts:

Fiore, A.M., et al., Geophys. Res. Lett., 33, L12809, doi:10.1029/2006GL026199, 2006.

Naik, V., et al., J. Geophys. Res., 110, D24306, doi:10.1029/2005JD005908, 2005.

Naik, V., et al., Geophys. Res. Lett., 34, L03818, doi:10.1029/2006GL028149, 2007.

West, J.J., et al., Geophys. Res. Lett., 34, L06806, doi:10.1029/2006GL029173, 2007.

West, J.J., et al., Proc. Natl. Acad. Sci., 103(11), 3988-3993, doi:10.1073/pnas.0600201103, 2006.

International assessments (IPCC AR4 and AEROCOM):

Dentener, F., et al., Global Biogeochem. Cycles, 20, GB4003, doi:10.1029/2005GB002672, 2006.

Dentener, F., et al., Environ. Sci. & Technol., 40, 3586-3594, 2006.

Ginoux, P., et al., J. Geophys. Res., 111, D22210, doi:10.1029/2005JD006707, 2006.

Horowitz, L.W., J. Geophys. Res., 111, D22211, doi:10.1029/2005JD006937, 2006.

Kinne, S., et al., Atmos. Chem. Phys., 6, 1815-1834, 2006.

Lamarque, J.-F., et al., J. Geophys. Res., 110, D08304, doi:10.1029/2004JD005537, 2005.

Shindell, et al., J. Geophys. Res., 111, 19306, doi:10.1029/2006JD007100, 2006.

Stevenson, D.S., et al., J. Geophys. Res., 111, D08301, doi:10.1029/2005JD006338, 2006.

Textor, C., et al., Atmos. Chem. Phys. Discuss., 7, 1699-1723, 2007.

Textor, C., et al., Atmos. Chem. Phys., 6, 1815-1834, 2006.

van Noije, T.P.C., et al., Atmos. Chem. Phys., 6, 2943-2979, 2006.

Field campaigns (ITCT-2k2 and ICARTT) and studies of biogenic hydrocarbons:

Cooper, O.R., et al., *J. Geophys. Res., 109*, D23S09, doi:10.1029/2003JD004006, 2004.

Fiore, A.M., et al., J. Geophys. Res., 110, D12303, doi:10.1029/2004jd005485, 2005.

Goldstein, A.H., et al., J. Geophys. Res., 109, D32S17, doi:10.1029/2003JD004406R, 2004.

Horowitz, L.W., et al., J. Geophys. Res., 112, D12S08, doi:10.1029/2006JD007747, 2007.

Mena-Carrasco, M., et al., J. Geophys. Res., in press, doi:10.1029/2006JD007762, 2007.

Tang, Y., et al., J. Geophys. Res., 109, D23S11, doi:10.1029/2004JD004513, 2004.

Tang, Y., et al., J. Geophys. Res., 112, D10S18, doi:10.1029/2006JD007515, 2007.

Real-time Air Quality Modeling System (RAQMS)

1. Brief description of model

Online unified troposphere/stratosphere global chemical data assimilation/forecasting system.

2. Principal applications or customers

Development of global satellite data chemical data assimilation capabilities; assessment of impacts of lateral boundary conditions, forecasting, and analysis support for airborne field missions.

3. Key participants, lab/organization, effort, contact information

R. Bradley Pierce, NOAA/NESDIS/STAR, brad.pierce@noaa.gov.

4. Literature citations, reports, or websites with detailed model description

Pierce, R.B., et al., Chemical data assimilation estimates of continental U.S. ozone and nitrogen budgets during INTEX-A, *J. Geophys. Res., accepted*, 2006.

Pierce, R.B., et al., Regional Air Quality Modeling System (RAQMS) predictions of the tropospheric ozone budget over east Asia, *J. Geophys. Res.*, 108, D218825, 2003.

Tang, Y., et al., Influence of lateral and top boundary conditions on regional air quality prediction: A multiscale study coupling regional and global chemical transport models, *J. Geophys. Res.*, 112, D10S18, doi:10.1029/2006JD007515, 2007.

Song, C.-K., et al., Downscale linkage of global model output for regional chemical transport modeling: Method and general performance, *J. Geophys. Res.*, *submitted*, 2007.

5. Specifications

Domain: Global.

Horizontal resolution and grid/coordinate system: Variable 1.4 x 1.4 to 2 x 2.5 latitude-longitude grid.

Vertical resolution and grid/coordinate system: 36 levels hybrid sigma-theta levels from the surface to ~60 km. Terrain following sigma coordinates transition to potential temperature in upper troposphere lower stratosphere (345-380 K).

Dynamical and numerical transport schemes: University of Wisconsin Hybrid Model dynamical core with CCM3 physics, transport uses flux form Piecewise Parabolic Method.

Chemistry and aerosol schemes: Chemistry: Family (O_x, NO_y, Cl_y, Br_y) approach with 55 transported species, fast species calculated using PCE assumptions. Standard O_x-HO_x-NO_x-ClO_x-BrO_x cycles governing the formation and destruction of odd oxygen, tropospheric NO_x-HO_x reactions, oxidation of CH₄, and CO. Treatment of Non-Methane HydroCarbons (NMHC) based on extended CB IV (explicit treatment of ethane, ethene, and methanol oxidation, semi-explicit treatment of propane) and explicit treatment of isoprene oxidation.

Planetary boundary layer and land-surface schemes: CCM3.

Deposition schemes: Surface deposition is computed according to the surface type and drag coefficients, with the calculation of the deposition rate modeled after Galbally and Roy [1980] and Levy et al. [1985]. Deposition velocities from Muller and Brasseur [1995]. Online wet removal of soluble species is based on convective fluxes and precipitation amounts [Liu et al., 2001; Park et al., 2004].

Sub-grid parameterizations: CCM3.

6. Sources of required data

Meteorological drivers/boundary conditions: NCEP GDAS meteorological analyses are used during chemical assimilation cycle.

Chemical boundary conditions/assimilations: Statistical Digital Filter (SDF) analysis system [Stobie 1985, 2000] to perform a univariate optimal interpolation (OI) global assimilation of satellite based O₃/CO profile and total column ozone observations.

Emission inventories and temporal/spatial processing: GEIA/EDGAR with updates for Asian emissions from Streets et al. [2003] and additional biogenic CO sources as described by Duncan et al. [2004]. Aircraft NO_x emissions are obtained from the HSRP database [*Stolarski et al.*, 1995]. Lightning NO_x emissions are calculated based on Price et al. [1997] and Pickering et al. [1998]. Biomass burning emissions use ecosystem/fire weather severity approach developed by Soja et al. [2004]. MODIS thermal anomaly data is used to provide area burned estimates. Fire severity is determined using the Haines index developed by the U.S. Forest Service.

7. Computational requirements

Hardware/software: Linux/Unix shared memory multi-processor platforms.

Simulation time: 2 x 2 degree 24hr assimilation cycle/5-day forecast cycle requires ~8hrs on 32 node SGI Origin 3000.

- Description of key outcomes, applications (including literature citations describing work), and other information about modeling capabilities
 - a. Literature Citations
 - Duncan, B.N., and I. Bey, A modeling study of the export pathways of pollution from Europe: Seasonal and interannual variations (1987–1997), *J. Geophys. Res.*, 109, D08301, doi:10.1029/2003JD004079, 2004.
 - Galbally, I.E., and C.R. Roy, Destruction of ozone at the earths' surface, O.J.R. Meteorol. Soc., 106, 599-620, 1980.
 - Levy, H. II, J.D. Mahlman, W.J. Moxim, and S.C. Liu, Tropospheric Ozone: The role of transport, *J. Geophys. Res.*, 90, 3735-3772, 1985.
 - Liu, H., D.J. Jacob, I. Bey, and R.M. Yantosca, Constraints from 210Pb and 7Be on wet deposition and transport in a global three-dimensional chemical tracer model driven by assimilated meteorological fields, *J. Geophys. Res.*, 106(D11), 12,109-12,128, 2001.
 - Muller, J.F., and G. Brasseur, IMAGES: A three dimensional chemical transport model of the global troposphere, *J. Geophys. Res.*, 100, 16,445-16,490, 1995.
 - Park, R.J., D.J. Jacob, B.D. Field, R.M. Yantosca, and M. Chin, Natural and transboundary pollution influences on sulfate-nitrate-ammonium aerosols in the United States: Implications for policy, *J. Geophys. Res.*, 109, D15204, doi:10.1029/2003JD004473, 2004.
 - Pickering, K.E., Y. Wang, W.-K. Tao, C. Price, and J.-F. Müller, Vertical distributions of lightning NO_x for use in regional and global chemical transport models, *J. Geophys. Res.*, 103(D23), 31,203-31,216, 1998.
 - Price, C., J. Penner, and M. Prather, NO_x from lightning: 1. Global distribution based on lightning physics, *J. Geophys. Res.*, 102(D5), 5929-5942, doi:10.1029/96JD03504, 1997.
 - Soja, A.J., W.R. Cofer, H.H. Shugart, A.I. Sukhinin, P.W. Stackhouse Jr., D. McRae, and S.G. Conard, Estimating fire emissions and disparities in boreal Siberia (1998 through 2002), *J. Geophys. Res.*, doi:10.1029/2004JD004570, 2004.
 - Stobie, J.M., et. al., The use of optimum interpolation at AFGWC, Proc., 7th Conference on Numerical Weather Prediction, Montreal, *Amer. Meteor. Soc.*, 43-49, 1985.
 - Stobie, J.M., Algorithm Theoretical Basis Document for Statistical Digital Filter (SDF) Analysis System (Stretch-Grid Version), Data Assimilation Office, NASA Goddard Space Flight Center, Greenbelt, Maryland, 20771, 2000.
 - Stolarski, R.S., S.L. Baughcan, W.H. Brune, A.R. Douglass, D.W. Fahey, R.R. Friedl, S.C. Liu, R.A. Plumb, L.R. Bole, H. Wesoky, and D.R. Worsnop, 1995 Scientific Assessment of the Atmospheric Effects of Stratospheric Aircraft, NASA Reference Publication 1381, 1995.
 - b. Key Outcomes and Applications
 - RAQMS is identified as a "primary existing system" for the "utilization of real-time air quality observations in regional air quality models" within the U.S. Group on Earth Observations (USGEO) Air Quality Assessment and Forecast Systems Near Term Opportunities (http://usgeo.gov/docs/nto/Air_Quality_NTO_2006-0925.pdf).

Development of assimilation capabilities using current satellite composition measurements (TOMS and OMI total column O_3 , HALOE, SAGE II, SAGE III solar occultation, and SAGE III limb scattering O_3 , profiles, and TES O_3 and CO profiles) to provide risk reduction for utilization of future operational NPP and NPOES composition measurements in global air quality forecasting.

Under the NASA ESE Atmospheric Composition focus area, RAQMS has been used in conjunction with Lagrangian trajectory models, satellite measurements, and aircraft data during the NASA 2001 TRACEP (Pierce et al., 2003), 2004 INTEX-A (Pierce et al., 2006), and 2006 INTEX-B and NOAA TEXAQS II airborne field missions to link aircraft, surface, and satellite observations through chemical data assimilation.

Under the NASA applied science program, RAQMS, chemical analyses have been used to:

- 1. Benchmark the impact of large-scale chemical boundary conditions on the USEPA's Community Multi-scale Air Quality (CMAQ) model (http://aiwg.gsfc.nasa.gov/esappdocs/benchmarks/AirQuality CMAQ Benchmark Final.pdf), and
- Develop capabilities to improve NOAA global air quality forecasting through development of a reduced chemical mechanism for incorporation into the NOAA GFS (http://aiwg.gsfc.nasa.gov/esappdocs/Air_Quality_FINAL_06.pdf).

2-D Middle Atmosphere Model (NOCAR)

1. Brief description of model

Coupled dynamical-radiative-chemical two-dimensional model of the middle atmosphere, including detailed ozone chemistry and its interaction with long and short lived gases.

2. Principal applications or customers

Evolution of ozone, ozone depletion potentials, lifetimes of source gases.

3. Key participants, lab/organization, effort, contact information

Robert Portmann, ESRL/CSD, robert.w.portmann@noaa.gov.

Susan Solomon, ESRL/CSD, susan.solomon@noaa.gov.

4. Literature citations, reports, or websites with detailed model description

Garcia et al., J. Geophys. Res., 97, 12,967-12,991, 1992.

Solomon et al., Geophys. Res. Lett., 25, 1871-1874, 1998.

Portmann et al., Geophys. Res. Lett., 26, 2387-2390, 1999.

5. Specifications

Domain: Zonal-mean, 90°S-90°N, 2-112 km.

Horizontal resolution and grid/coordinate system: 5.11° (36 bins).

Vertical resolution and grid/coordinate system: 2 km (56 bins).

Dynamical and numerical transport schemes: Transformed Eulerian-Mean including planetary wave and gravity wave

breaking.

Chemistry and aerosol schemes: Detailed family chemistry.

Planetary boundary layer and land-surface schemes: NA

Deposition schemes: NA

Sub-grid parameterizations: Gravity wave breaking, diffusion.

6. Sources of required data

Meteorological drivers/boundary conditions: NCEP Wave 1-3 amplitudes. Chemical boundary conditions/assimilations: SRES emission scenarios.

Emission inventories and temporal/spatial processing: NA

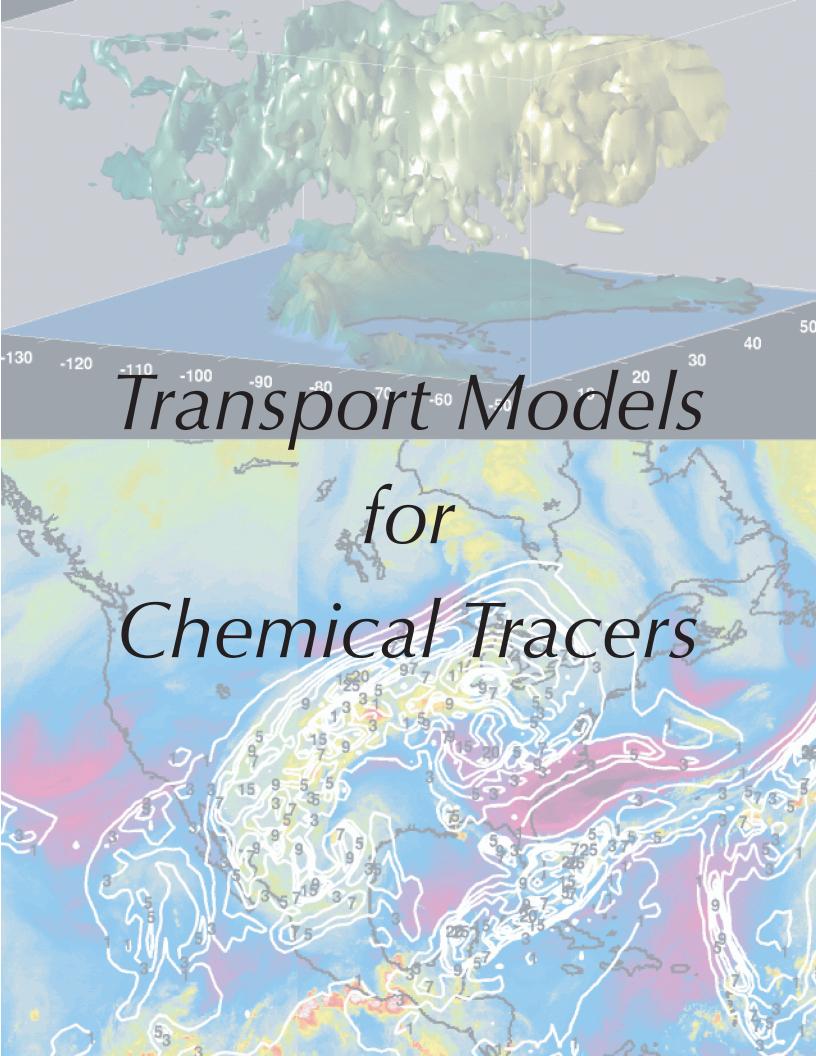
7. Computational requirements

Hardware/software: Any workstation, FORTRAN90.

Simulation time: Variable, e.g., 30 min/year.

- 8. Description of key outcomes, applications (including literature citations describing work), and other information about modeling capabilities
 - a. Evolution of Ozone: Elucidating the effect of volcanic aerosols on the evolution of ozone and their effect on ozone photochemistry.
 - Solomon, S., R.W. Portmann, R.R. Garcia, L.W. Thomason, L.R. Poole, and M.P. McCormick, The role of aerosol variations in anthropogenic ozone depletion at northern midlatitudes, *J. Geophys. Res.*, 101, 6713-6727, 1996.
 - Portmann, R.W., S. Solomon, R.R. Garcia, L.W. Thomason, L.R. Poole, and M.P. McCormick, Role of aerosol variations in anthropogenic ozone depletion in polar regions, *J. Geophys. Res.*, 101, 22,991-23,006, 1996.
 - Solomon, S., R.W. Portmann, R.R. Garcia, W. Randel, F. Wu, et al., Ozone depletion at mid-latitudes: Coupling of volcanic aerosols and temperature variability to anthropogenic chlorine, *Geophys. Res. Lett.*, 25, 1871-1874, 1998.
 - b. Role of NO_x in the stratosphere: Evaluations of the effect of NO_x on stratospheric photochemistry including its effect on other ozone destroying catalytic cycles and ozone trends.

- Nevison, C.D., S. Solomon, and R.S. Gao, Buffering interactions in the modeled response of stratospheric O₃ to increased NO₂ and HO₂, *J. Geophys. Res.*, 104, 3741-3754, 1999.
- Portmann, R.W., S.S. Brown, T. Gierczak, R.K. Talukdar, J.B. Burkholder, and A.R. Ravishankara, Role of nitrogen oxides in the stratosphere: A reevaluation based on laboratory studies, *Geophys. Res. Lett.*, 26, 2387-2390, 1999.
- c. Stratospheric bromine photochemistry: Studies which estimate the effectiveness of bromine on stratospheric ozone by its direct photochemical effect and due to the enhanced conversion of its source gases.
 - Daniel, J.S., S. Solomon, R.W. Portmann, and R.R. Garcia, Stratospheric ozone destruction: The importance of bromine relative to chlorine, *J. Geophys. Res.*, 104, 23,871-23,880, 1999.
 - Dvortsov, V.L., M.A. Geller, S. Solomon, S.M. Schauffler, E.L. Atlas, and D.R. Blake, Rethinking reactive halogen budgets in the midlatitude lower stratosphere, *Geophys. Res. Let.*, 26, 1699-1702, 1999.
- d. Ozone depletion potenials (ODP) and global warming potentials (GWP): Evaluating the definition of ODPs and estimating the ODPs and GWPs of several source gases.
 - Solomon, S., A.F. Tuck, M. Mills, L.E. Heidt, and W.H. Pollock, On the evaluation of ozone depletion potentials, *J. Geophys. Res.*, 97, 825–842, 1992.
 - Solomon, S., J.B. Burkholder, A.R. Ravishankara, and R.R. Garcia, Ozone depletion and global warming potentials of CF₃I, *J. Geophys. Res.*, 99, 20,929-20,935, 1994.
 - Portmann, R.W., and S. Solomon, Indirect radiative forcing of the ozone layer during the 21st century, *Geophys. Res. Let.*, 34, L02813, doi:10.1029/2006GL028252, 2007.
- e. Other topics on ozone chemistry: Exploratory papers which study possible effects on ozone by new processes (e.g., cirrus clouds and iodine containing compounds).
 - Solomon, S., S. Borrmann, R.R. Garcia, R. Portmann, L. Thomason, L.R. Poole, D. Winker, and M.P. McCormick, Heterogeneous chlorine chemistry in the tropopause region, *J. Geophys. Res.*, 102, 21,411-21,429, 1997.
 - Solomon, S., R.R. Garcia, and A.R. Ravishankara, On the role of iodine in ozone depletion, *J. Geophys. Res.*, 99, 20,491-20,499, 1994.



Transport Model 5 (TM5) / CarbonTracker

1. Brief description of model

An offline tracer transport model using 3-hourly ECMWF meteorology to simulate global tracer distributions. Uses two-way nesting to zoom in to 1 x 1 degree for areas of interest.

2. Principal applications or customers

Global to regional chemical composition studies, CarbonTracker.

3. Key participants, lab/organization, effort, contact information

ESRL/GMD Carbon Tracker team: Wouter Peters (wouter.peters@noaa.gov), Andy Jacobson (andy.jacobson@noaa.gov).

4. Literature citations, reports, or websites with detailed model description

Krol, M., et al., The two-way nested global chemistry-transport zoom model TM5: algorithm and applications, *Atmos. Chem. Phys.*, *5*(2), 417-432, 2005.

Peters, W., et al., Toward regional-scale modeling using the two-way nested global model TM5: Characterization of transport using SF₆, *J. Geophys. ReS.*, 109(D19), D19314, 2004.

http://www.esrl.noaa.gov/gmd/ccgg/carbontracker/.

5. Specifications

Domain: Global, two-way nested.

Horizontal resolution and grid/coordinate system: 3 x 2 degrees with nesting up to 1 x 1 degrees.

Vertical resolution and grid/coordinate system: Choice of 25, 34, 60, or 91 level hybrid sigma-pressure up to top of atmosphere.

Dynamical and numerical transport schemes: Slopes or second moments advection scheme with two-way nested zoom (Prather, M., Numerical advection by conservation of second-order moments, *J. Geophys. Res.*, *91*, 6671-6681, 1986; Russell, G., and J. Lerner, A new finite-differencing scheme for the tracer transport equation, *J. Appl. Meteorol.*, *20*, 1483-1498; Petersen, A.C., et al., An evaluation and intercomparison of four new advection schemes for use in global chemistry models, *J. Geophys. Res.*, *103*(D15), 19,253-19,269, 1998.; Berkvens et al., 2001).

Chemistry and aerosol schemes: CBM-4 (gases), M7 (aerosols), tailor made schemes (SF₆, 222Rn, MCF, etc.).

Planetary boundary layer and land-surface schemes: Follows ECMWF code: Beljaars and Viterbo (1999); Vogelezang and Holtslag (1996); Holtslag and Boville (1993); Louis, J.F., A parametric model of vertical eddy fluxes in the atmosphere, *Boundary Layer Meteorol.*, 17, 187-202, 1979.

Deposition schemes: Gases: Wesley (1989) and Ganzeveld et al. (2003).

Sub-grid parameterizations: Tiedtke, M., A comprehensive mass flux scheme for cumulus parameterization in large-scale models, *Mon. Wea. Rev., 117*(8), 1779-1800, 1989, for convective fluxes (shallow, deep convection).

6. Sources of required data

Meteorological drivers/boundary conditions: European Centre for Medium Range Weather Forecasting (ERA40 or operational forecast) or NCEP (reanalysis or GFS forecast).

Chemical boundary conditions/assimilations: TOMS stratospheric O₃, GMD CO₂ data. TM5 is equipped with both an ensemble Kalman filter assimilation framework and a 4-D-variational scheme based on its full adjoint code.

Emission inventories and temporal/spatial processing: Multiple sources: EDGAR, EPA, GEIA, etc.

7. Computational requirements

Hardware/software: Implemented on range of platforms around the world (several linux clusters, CRAY, IBM, Fujitsu, OSX). Simulation time: Variable: Example for CarbonTracker is 1.5 hour per week of assimilation when using two nested regions (6 x 4, 3 x 2, 1 x 1 resolutions).

- 8. Description of key outcomes, applications (including literature citations describing work), and other information about modeling capabilities
 - a. CarbonTracker: TM5 underlies the operational reanalysis of global CO₂ surface sources and sinks with a focus on North

- America. Available at http://www.carbontracker.noaa.gov.
- Peters et al., Proc. Natl. Acad. Sci., submitted, U.S., 2--7.
- b. IPCC: TM5 is one of the models used in the current IPCC assessment of ozone and air quality, IPCC (2007). Stevenson, D.S., et al., *J. Geophys. Res.*, 111, 2006.
- c. EverGreen and TransCom Continuous: TM5 was recently compared to a suite of other models used in the EU project EverGreen aimed at operational assimilations of methane and carbon dioxide. TM5 has four different sets of output represented the international TransCom continuous intercomparison study focusing on the simulation of high frequency continental trace gas observations.

Bergamaschi et al., ISBN 92-79-02001-3, 53 pp., 2006.

- Law et al., Atmos. Chem. Phys., submitted, 2007.
- d. Global methane budget, 4-D-VAR: TM5 was used to check reported methane emissions in the EU based on inverse modeling and 4-D-var data assimilation.
 - Bergamaschi et al., Atmos. Chem. Phys., 5, 2431-2460, 2005.
 - Houweling, S., et al., Geophys. Res. Lett., 33, 2006.
- e. Ongoing methyl chloroform emissions: TM5 was used to check for ongoing methyl chloroform emissions, a substance controlled under the Montreal Protocol. Krol, M., et al., Continuing emissions of methyl chloroform from Europe, *Nature*, *421*, 131-135, 2003.
- f. Remote Sensing: TM5 is used extensively to evaluate new remote sensing products from SCIAMACHY, AIRS, and GOME. Active modeling of NO₂, CO, CH₄, CO₂, and HCHO columns is ongoing.

Van Noie et al., Atmos. Chem. Phys., 6, 2943-2979, 2006.

- de Laat et al., Geophys. Res. Lett., 33, 2006.
- Straume, A.G., et al., Adv. Space Res., 36, 821-827, 2005; Gloudemans, A.M.S., et al., Geophys. Res. Lett., 33, 2006.
- g. Stratospheric Studies: TM5 is used to study stratospheric composition and recovery of the ozone layer.
 - van Noije et al., J. Geoph. Res., doi:10.1029/2005JD006081, 2006.
 - Bregman et al., Atmos. Chem. Phys., 6(12), 4529-4543, 2006.
- h. Additional References:
 - Olivié, D.J.L., *On the role of convection and turbulence for tropospheric ozone and its precursors*, PhD thesis, Technical University of Eindhoven, The Netherlands, 2005.
 - Olivié, D.J.L., P.F.J. van Velthoven, and A.C.M. Beljaars, Evaluation of archived and off-line diagnosed vertical diffusion coefficients from ERA-40 with Rn simulations, *Atmos. Chem. Phys.*, 4(9/10):2313-2336, 2005.
 - Peters, W., TM5 manual for parallel version, Research document, 2003.
 - Segers, A., et al., On the computation of mass fluxes for Eulerian transport models from spectral meteorological fields, in *Proc. of the 2002 Intl. Conf. on Computational Sci., vol. 2330/2002* of *Lecture Notes in Computer Sci.*, pages 767-776, Springer Verlag, 2002.
 - van den Broek, M.M.P., A. Bregman, and J. Lelieveld, Model study of stratospheric chlorine activation and ozone loss during the 1996/1997 winter, *J. Geophys. Res.*, 105(D23), 28,961-28,978, 2000.
 - van den Broek, M.M.P., M.K. van Aalst, A. Bregman, M. Krol, J. Lelieveld, G.C. Toon, S. Garcelon, G.M. Hansford, R.L. Jones, and T.D. Gardiner, The impact of model grid zooming on tracer transport in the 1999/2000 arctic polar vortex, *Atmos. Chem. Phys.*, *3*(5), 1833-1847, 2003.
 - van den Broek, M.M.P., J.E. Williams, and A. Bregman, Implementing growth and sedimentation of nat particles in a global eulerian model, *Atmos. Chem. Phys.*, 4(7), 1869-1883, 2004.
 - van Noije, T.P.C., H.J. Eskes, M. van Weele, and P.F.J. van Velthoven, Implications of the enhanced Brewer-Dobson circulation in European Centre for Medium-Range Weather Forecasts reanalysis ERA-40 for the stratosphere-troposphere exchange of ozone in global chemistry transport models, *J. Geophys. Res.*, 109(D19):D19308, 2004.
 - Williams, J., J. Landgraf, A. Bregman, and H. Walter, A modified band approach for the accurate calculation of online photolysis rates in stratospheric-tropospheric chemistry transport models, *Atmos. Chem. Phys.*, 6(12), 4137-4161, 2006.

FLEXPART

1. Brief description of model

A Lagrangian particle dispersion model for use on global to regional scales.

2. Principal applications or customers

Used for diagnosing the intercontinental and regional scale transport of emissions from area or point sources in greater detail than is typically possible with Eulerian models. The model is currently used by 34 groups at universities or research laboratories in 17 countries. The model can simulate the forward transport of emissions, or the backward transport of an airmass from a given receptor site, using thousands of back trajectories in what is known as a retroplume.

3. Key participants, lab/organization, effort, contact information

Owen Cooper, CIRES/NOAA ESRL, fulltime, owen.r.cooper@noaa.gov.

4. Literature citations, reports, or websites with detailed model description

Users manual: Stohl, A., C. Forster, A. Frank, P. Seibert, and G. Wotawa, Technical Note: The Lagrangian particle dispersion model FLEXPART version 6.2., *Atmos. Chem. Phys.*, 5, 2461-2474, 2005.

Website: http://transport.nilu.no/flexpart.

5. Specifications

Domain: Global to regional scale, as specified by the user.

Horizontal resolution and grid/coordinate system: Typically 1 x 1 degree for global but higher resolution wind fields from mesoscale models like WRF can also be used.

Vertical resolution and grid/coordinate system: Typically 91 levels for ECMWF data and 26 levels for GFS data. Higher resolution is certainly possible. Can be used with eta or pressure surfaces, but the model runs on eta surfaces.

Dynamical and numerical transport schemes: Lagrangian particle advection using 3-D winds at 15 minute timesteps, although shorter timesteps can be specified.

Chemistry, and aerosol schemes: No chemistry, although e-folding lifetimes to the tracers can be imposed.

Planetary boundary layer and land-surface schemes: Particles are redistributed vertically within the boundary layer according to the surface sensible heat fluxes and friction velocity. A global landuse database is used in this paramaterization.

Deposition schemes: Wet and dry deposition schemes can be implemented.

Sub-grid parameterizations: The model has a sub-grid convection parameterization based on the work of Emanuel and Živković-Rothman, Development and evaluation of a convection scheme for use in climate models, *J. Atmos. Sci.*, 56, 1766-1782, 1999.

6. Sources of required data

Meteorological drivers/boundary conditions: ECMWF or GFS analyses with 3-hour forecasts.

Chemical boundary conditions/assimilations: None.

Emission inventories and temporal/spatial processing: Various. Most commonly used global anthropogenic emissions come from the 2000 EDGAR inventory. U.S. emissions typically come from the EPA 1999 inventory with recent updates to the point sources.

7. Computational requirements

Hardware/software: A single LINUX or UNIX machine and a FORTRAN77 compiler.

Simulation time: A one-month forward simulation using 20 million particles takes about 4-5 days. A backward (retroplume) simulation using 1.3 million particles takes about 4 hours.

 Description of key outcomes, applications (including literature citations describing work), and other information about modeling capabilities

FLEXPART has been used in over 100 published studies of the global and regional transport of various trace gases and particulate matter (see publication list at http://zardoz.nilu.no/~andreas/flextra+flexpart.html). At NOAA ESRL the model has

been used to identify the transport of plumes from Asia to North America and from North America to Europe. Its most recent application has been to provide highly detailed simulations of stratospheric intrusions and lightning NO_x emissions. The Lagrangian nature of the model allows trajectory particle to be released from the exact location of all lightning flashes detected by the National Lightning Detection Network above North America during a given summer.

- Cooper, O.R., A. Stohl, M. Trainer, A. Thompson, J.C. Witte, S.J. Oltmans, G. Morris, K.E. Pickering, J.H. Crawford, G. Chen, R.C. Cohen, T.H. Bertram, P. Wooldridge, A. Perring, W.H. Brune, J. Merrill, J.L. Moody, D. Tarasick, P. Nédélec, G. Forbes, M.J. Newchurch, F.J. Schmidlin, B.J. Johnson, S. Turquety, S.L. Baughcum, X. Ren, F.C. Fehsenfeld, J.F. Meagher, N. Spichtinger, C.C. Brown, S.A. McKeen, I.S. McDermid, and T. Leblanc, Large upper tropospheric ozone enhancements above mid-latitude North America during summer: In situ evidence from the IONS and MOZAIC ozone monitoring network, J. Geophys. Res., 111, D24S05, doi:10.1029/2006JD007306, 2006.
- Cooper, O.R., A. Stohl, G. Hübler, E.Y. Hsie, D.D. Parrish, A.F. Tuck, G.N. Kiladis, S.J. Oltmans, B.J. Johnson, M. Shapiro, J.L. Moody, and A.S. Lefohn, Direct transport of mid-latitude stratospheric ozone into the lower troposphere and marine boundary layer of the tropical Pacific Ocean, *J. Geophys. Res.*, 110, D23310, doi:10.1029/2005JD005783, 2005.
- Cooper, O.R., A. Stohl, S. Eckhardt, D.D. Parrish, S.J. Oltmans, B.J. Johnson, P. Nedelec, F.J. Schmidlin, M.J. Newchurch, Y. Kono, and K. Kita, A springtime comparison of tropospheric ozone and transport pathways on the east and west coasts of the United States, *J. Geophys. Res.*, 110, D05S90, doi:10.1029/2004JD005183, 2005.
- Cooper, O.R., M. Trainer, A.M. Thompson, S.J. Oltmans, D.W. Tarasick, J.C. Witte, A. Stohl, S. Eckhardt, J. Lelieveld, M.J. Newchurch, B.J. Johnson, R.W. Portmann, L. Kalnajs, M.K. Dubey, T. Leblanc, I.S. McDermid, G. Forbes, D. Wolfe, T. Carey-Smith, G.A. Morris, B. Lefer, B. Rappenglück, E. Joseph, F. Schmidlin, J. Meagher, F.C. Fehsenfeld, T.J. Keating, R.A. Van Curen, and K. Minschwaner, Evidence for a recurring eastern North America upper tropospheric ozone maximum during summer, *J. Geophys. Res., in press*, 2007.

Stochastic Time-Inverted Lagrangian Transport (STILT)

1. Brief description of model

Lagrangian particle dispersion model.

2. Principal applications or customers

Interpreting greenhouse gas measurements.

3. Key participants, lab/organization, effort, contact information

Adam Hirsch, NOAA/ESRL GMD, adam.hirsch@noaa.gov.

Arlyn Andrews, NOAA/ESRL GMD, arlyn.andrews@noaa.gov.

4. Literature citations, reports, or websites with detailed model description

Lin, J.C., C. Gerbig, S.C. Wofsy, et al., A near-field tool for simulating the upstream influence of atmospheric observations: The Stochastic Time-Inverted Lagrangian Transport (STILT) model, *J. Geophy. Res.*, 108(D16), 4493, doi:10.1029/2002JD003161, 2003.

5. Specifications

Domain: 145W to 50W, 11N to 65N high resolution nested grid.

Horizontal resolution and grid/coordinate system: Depends on driving meteorology.

Vertical resolution and grid/coordinate system: Depends on driving meteorology; typically lat-lon.

Dynamical and numerical transport schemes: Lagrangian – 3 hour winds interpolated to particle positions.

Chemistry and aerosol schemes: None.

Planetary boundary layer and land-surface schemes: Hanna (1982); Vogelezang and Holtslag for PBL height (1996).

Deposition schemes: None.

Sub-grid parameterizations: Moist convection uses Grell-Devenyi when driven by RAMS meteorology.

6. Sources of required data

Meteorological drivers/boundary conditions: Can be driven by NCEP NAM, nested in NCEP FNL; can also use RAMS and WRF, as long as output is converted to ARL format.

Chemical boundary conditions/assimilations: $NA - exploring using CarbonTracker 4-D CO_2$ fields as a boundary condition for regional runs.

Emission inventories and temporal/spatial processing: Depends on preference of user.

7. Computational requirements

Hardware/software: R and FORTRAN.

Simulation time: Depends on resolution and number of particles.

 Description of key outcomes, applications (including literature citations describing work), and other information about modeling capabilities

Mainly we are using this model and FLEXPART for forward runs to test CO₂ flux inventories and also to generate surface influence functions for inverse modeling.

Important opportunities for synergy between ESRL GMD and other groups that would vastly improve the utility of these models for use as chemical transport models:

- 1. Archiving of subgrid convective fluxes in WRF-NAM or RUC. Currently, for STILT to simulate moist convection in a believable manner, special WRF or RAMS runs must be done. Now that WRF is being used for NAM forecasting at very high spatial resolution and is being archived it would be a tremendous resource if the variables needed to parameterize moist convection in STILT (or even the mass fluxes directly from the WRF runs) were available.
- 2. Currently the highest resolution that FLEXPART can be run with archived meteorology is 1 degree (ECMWF or NCEP GFS). However, FLEXPART can also be driven by WRF winds. The capability to run FLEXPART off of archived WRF-NAM, NARR, or RUC would be a tremendous help. Otherwise, we would again have to collaborate with others to run WRF (which we would also be happy to do if this were possible!).

Hybrid Single Particle Lagrangian Integrated Trajectory (HYSPLIT)

1. Brief description of model

A complete off-line system for computing simple air parcel trajectories to complex dispersion and deposition simulations.

2. Principal applications or customers

Air quality data analysis, source attribution; NOAA for smoke forecast tool and emergency response such as volcanic eruptions, nuclear accidents (supporting WMO), and homeland security incidents; DoD, CMA (Canada), BoM (Australia), university researchers, and available interactively on-line.

3. Key participants, lab/organization, effort, contact information

Roland Draxler, OAR/ARL, roland.draxler@noaa.gov.

4. Literature citations, reports, or websites with detailed model description

Draxler, R.R., and G.D. Hess, An overview of the HYSPLIT-4 modeling system for trajectories, dispersion, and deposition, *Aust. Met. Mag.*, 47, 295-308, 1998.

Draxler, R.R., and G.D. Hess, Description of the HYSPLIT-4 modeling system, NOAA Tech Memo ERL ARL-224, Dec, 24 pp., 1997.

http://www.arl.noaa.gov/hysplit.

5. Specifications

Domain: Local scale (5 km) to global scale (depends upon the input meteorology).

Horizontal resolution and grid/coordinate system: Identical to the input meteorological data; multiple nested grids, each with different resolutions and coordinate systems are permitted.

Vertical resolution and grid/coordinate system: All meteorological data remapped to a terrain following coordinate system at the resolution of the input meteorological data.

Dynamical and numerical transport schemes: Lagrangian solution of the advection-diffusion equation.

Chemistry and aerosol schemes: Optional modules for $SO_2 \rightarrow SO_4$, ozone formation (IER, GRS, CB-IV; see http://www.arl.noaa.gov/ready/hyspchem/), and specialized versions for mercury, dioxin, atrazine (see http://www.arl.noaa.gov/ss/transport/cohen.html).

Planetary boundary layer and land-surface schemes: Surface-layer similarity based upon wind and temperature profiles if turbulent fluxes or TKE not available from the input meteorological data.

Deposition schemes: Explicit removal or resistance based on Wesley (1989) and Slinn & Slinn (1980).

Sub-grid parameterizations: Smagorinsky deformation for horizontal turbulence; Lumley-Panofsky for TKE anisotropy, or based on wind and temperature profiles.

6. Sources of required data

Meteorological drivers/boundary conditions: Drivers available for WRF-NMM, WRF-ARW, LAPS, MM5, RAMS, COAMPS, GFS, HIRLAM, ECMWF, MUP.

Chemical boundary conditions/assimilations: NESDIS HMS and AOD; NASA TOMS.

Emission inventories and temporal/spatial processing: Interface available through CMAQ.

7. Computational requirements

Hardware/software: Multiple: UNIX and LINUX (single processor and cluster versions), Windows-XP, and MAC-OSX.

Simulation time: 90-sec wall-clock for a 1-day simulation per 10,000 particles on a 2.8 Ghz single processor Xeon PC using the NAM 12 km meteorological data, 5 km concentration grid.

 Description of key outcomes, applications (including literature citations describing work), and other information about modeling capabilities

Wildfire Smoke Forecasting – http://www.weather.gov/aq/sectors/conus.php.

Dust Storms - Escudero, M., et al., Determination of the contribution of northern Africa dust source areas to PM₁₀ concentra-

- tions over the central Iberian Peninsula using the Hybrid Single-Particle Lagrangian Integrated Trajectory (HYSPLIT) model, *J. Geophys. Res.*, 111, D06210, doi:10.1029/2005JD006395; Estimating PM₁₀ air concentrations from dust storms in Iraq, Kuwait, and Saudi Arabia, *Atmos. Environ.*, 35, 4315-4330.
- Mercury fate and transport Cohen, M., et al., Modeling the atmospheric transport and deposition of PCDD/F to the Great Lakes, *Environ. Sci. Tech.*, *36*, 4831-4845, 2002.
- Dioxin fate and transport Cohen, M., et al., Modeling the atmospheric transport and deposition of mercury to the Great Lakes, *Environ. Res.*, *95*, 247-265, 2004.
- Ozone Chemistry Stein, A.F., D. Lamb, and R.R. Draxler, Incorporation of detailed chemistry into a three-dimensional Lagrangian-Eulerian hybrid model: Application to regional tropospheric ozone, *Atm. Environ.*, *34*, 4361-4372, 2000.
- Emergency Response Draxler, R.R., M. Jean, B. Hicks, and D. Randerson, *Emergency preparedness Regional Specialized Meteorological Centers at Washington and Montreal: Radiation Protection Dosimetry*, 73, 27-30, 1997.
- Trajectory Analysis Harris, J.M., R.R. Draxler, and S.J. Oltmans, Trajectory model sensitivity to differences in input data and vertical transport method, *J. Geophys. Res.*, 110, D14109, doi:10.1029/2004JD005750, 2005.
- Ensemble Forecasting Draxler, R.R., Evaluation of an ensemble dispersion calculation, J. Appl. Meteorol., 42, 308-317, 2001.
- Urban Dispersion Draxler, R.R., The use of global and mesoscale meteorological model data to predict the transport and dispersion of tracer plumes over Washington, D.C., *Weather and Forecasting*, 21(3), 383-394, 2006.
- Volcanic Eruptions Heffter, J.L., and B.J.B. Stunder, Volcanic Ash Forecast Transport And Dispersion (VAFTAD) Model, *Weather and Forecasting, 8*, 534-541, 1993, see products posted at http://www.ssd.noaa.gov/VAAC/vaftad.html and http://weather.noaa.gov/fax/wafsash.shtml.

Global Chemical Transport Model - Dust and Dissolved Iron (GCTM-Dust)

1. Brief description of model

Global transport of dust undergoing chemical reactions leading to acid coating and subsequent dissolution of ferric minerals.

2. Principal applications or customers

Provides dissolved iron (bio-available Fe) deposition to ocean biogeochemical models.

3. Key participants, lab/organization, effort, contact information

Song-Miao Fan, GFDL, full-time, songmiao.fan@noaa.gov.

Walter Moxim, GFDL, full-time.

Hiram Levy, GFDL full-time.

4. Literature citations, reports, or websites with detailed model description

Fan, et al., Geophys. Res. Lett., 33; ftp://ftp.agu.org/apend/gl/2005gl024852, 2006.

Mahlman and Moxim, J. Atmos. Sci., 35, 1340-1374, 1978.

5. Specifications

Domain: Global.

Horizontal resolution and grid/coordinate system: Equal area grid at 265 km.

Vertical resolution and grid/coordinate system: 28 levels matching the NCEP re-analysis model.

Dynamical and numerical transport schemes: Fourth order in the vertical and second order in the horizontal.

Chemistry and aerosol schemes: ftp://ftp.agu.org/apend/g1/2005g1024852.

Planetary boundary layer and land-surface schemes: NCEP re-analysis.

Deposition schemes: Dry deposition adapted from Giorgi (1986), Wet deposition adapted from Kasibhatla et al. (1991).

Sub-grid parameterizations: Adapted from Levy et al. (1982).

6. Sources of required data

Meteorological drivers/boundary conditions: NCEP re-analysis.

Chemical boundary conditions/assimilations: None.

Emission inventories and temporal/spatial processing: Spatial distribution of dust sources: Ginoux et al. (2001), Dust entrainment: Marticorena and Bergametti (1995).

7. Computational requirements

Hardware/software: 6 CPUs on the GFDL HPCS. FORTRAN90.

Simulation time: 12 hours wall-clock for 1-year simulation using 16 tracers for dust mass and life stages (fresh, coated, and dissolved).

8. Description of key outcomes, applications (including literature citations describing work), and other information about modeling capabilities

Present ocean biogeochemistry models assume constant solubility for aeolian dust iron deposition, even though measurements have shown large variability of aerosol iron solubility (generally increasing with transport time and decreasing with dust concentration). In the GFDL Global Chemical Transport Model, the variable aerosol iron solubility is predicted by explicitly considering chemical and cloud processes that lead to acid coating on desert dust aerosols followed by dissolution of ferric minerals. The model thus simulates a more realistic atmospheric input of bio-available iron to the global ocean, an important boundary condition for the ocean biogeochemistry models.

Fan, S., L.W. Horowitz, W.J. Moxim, and H. Levy II, Impact of air pollution on wet deposition of mineral dust aerosols, *Geophys. Res. Lett.*, 31, L02104, doi:10.1029/2003GL018501, 2004.

Fan, S., W.J. Moxim, and H. Levy II Aeolian input of bioavailable iron to the ocean, *Geophys. Res. Lett.*, 33, L07602, doi:10.1029/2005GL024852, 2006.

Rapid Update Cycle / Colorado State University Lagrangian Particle Dispersion Model (RUC/CSU-LPDM)

1. Brief description of model

RUC: Regional mesoscale model used for hourly assimilation/model forecasts, used operationally at NCEP for aviation, severeweather, and other situational awareness applications. Hourly 3-D grids used for CSU-LPDM application.

CSU-LPDM: Backward trajectory model that calculates concentrations of species released at a receptor in the modeling domain. The model can use RUC or other regional model output to calculate wind and its turbulent components. For this purpose Markov chain type equations are employed. Interaction of species with surface is also parameterized.

2. Principal applications or customers

NCEP operational model for aviation, severe weather, situational awareness. Used extensively for observation assessment studies (e.g., profiler, aircraft, GPS precipitable water). Research applications with NASA for aviation work, DOE for wind energy forecasting, regional experimental applications (e.g., Hydrometeorological Testbed – HMT).

LPDM can be applied to any source-receptor modeling ranging from carbon cycle source attribution to emergency response applications (e.g., release of radionuclides, toxins, etc.).

3. Key participants, lab/organization, effort, contact information

RUC: ESRL/GSD Assimilation and Modeling Branch – Stan Benjamin.

CSU-LPDM: Marek Uliasz - Colo. State Univ., Mariusz Pagowski - ESRL/GSD.

4. Literature citations, reports, or websites with detailed model description

RUC: Benjamin et al., Mon. Wea. Rev., 2 companion articles, 2004.

CSU-LPDM: Uliasz, M., Lagrangian particle modeling in mesoscale applications, *Environ. Modeling*, ed. P. Zanetti, Computational Mechanics, Publications, 71-102, 994.

5. Specifications

Domain: Regional.

Horizontal resolution and grid/coordinate system: Variable resolution – tested from 10-60 km resolution; resolution from tens of meters upwards.

Vertical resolution and grid/coordinate system: Variable resolution, isentropic-sigma, currently at 50 levels; variable, terrain following.

Dynamical and numerical transport schemes: Flux-corrected transport, Lagrangian, Markov chain wind.

Chemistry and aerosol schemes: None.

Planetary boundary layer and land-surface schemes: Burk Thompson PBL, RUC-Smirnova land-surface, turbulent variances derived from turbulent kinetic energy supplied by the meteorological driver or derived from wind/temperature profiles.

Deposition schemes: None currently; Monin, A., On the boundary condition on the earth surface for diffusing pollution, *Adv. Geophys.*, 6, 435-436, 1959.

Sub-grid parameterizations: Grell-Devenyi ensemble closure convective parameterization scheme, convective transport of species in development, PBL as described above.

6. Sources of required data

Meteorological drivers/boundary conditions: RUC: Extensive data assimilation system for RUC, boundary conditions from NAM or GFS; CSU-LPDM: RAMS, other regional models can easily be implemented.

Chemical boundary conditions/assimilations: None.

Emission inventories and temporal/spatial processing: None.

7. Computational requirements

Hardware/software: Runs on multiple-processor allotments on ijet/wjet/ejet; parallelized over different receptors, runs on any windows/linux PC.

Simulation time: 100 processors 72 hour forecast, 13 km-50 levels, 451 x 337 grid, 100 minutes.

8. Description of key outcomes, applications (including literature citations describing work), and other information about modeling capabilities

For applications of LPDM, see http://users.frii.com/uliasz/modeling/publ.htm.

Infusing satellite Data into Environmental Applications (IDEA)

1. Brief description of model

48-hour aerosol trajectory forecasts, initialized from regions of enhanced aerosol optical depth (AOD) observed by MODIS on the NASA Terra satellite, are combined with MODIS Direct Broadcast AOD imagery, surface PM_{2.5} observations from EPA AIRNOW, and GOES WF-ABBA fire locations to provide information to air quality forecasters.

2. Principal applications or customers

Satellite based PM_{2.5} forecast guidance for regional air quality forecasters.

3. Key participants, lab/organization, effort, contact information

IDEA was developed at NASA Langley Research Center in partnership with EPA and NOAA under the NASA Applied Sciences Program. IDEA was transferred to CIMSS in 2004 and has been in continuous operation since April 2004. IDEA is currently being transferred from CIMSS to NOAA/NESDIS under a NASA Applied Sciences Program grant to the University of Maryland-Baltimore County (Ray Hoff, UMBC, PI).

NOAA POC: Shobha Kondragunta, NOAA/NESDIS/STAR, shobha.kondragunta@noaa.gov.

4. Literature citations, reports, or websites with detailed model description

Al-Saadi, J.A., et al., Improving national air quality forecasts with satellite aerosol observations, *Bull. Amer. Meteor. Soc.*, 86, 1249-1261, 2005.

NASA Benchmark report: http://aiwg.gsfc.nasa.gov/esappdocs/benchmarks/AQI benchmark report v16.doc.

Website: http://idea.ssec.wisc.edu/.

5. Specifications

Domain: Continental U.S.

Horizontal resolution and grid/coordinate system: 40-km Lambert Conformal grid (12Z NOAA/NCEP NAM forecast GRIB 212 data).

Vertical resolution and grid/coordinate system: Mandatory Pressure levels (12Z NOAA/NCEP NAM forecast GRIB 212 data).

Dynamical and numerical transport schemes: 4th order Runge-Kutta trajectories.

Chemistry and aerosol schemes: None.

Planetary boundary layer and land-surface schemes: None.

Deposition schemes: None.

Sub-grid parameterizations: None.

6. Sources of required data

Meteorological drivers/boundary conditions: 12Z NOAA/NCEP NAM forecast GRIB 212 data.

Chemical boundary conditions/assimilations: MODIS Terra AOD from CIMSS Direct Broadcast, surface PM_{2.5} measurements from EPA AIRNOW, fire locations from GOES WF-ABBA.

Emission inventories and temporal/spatial processing: None.

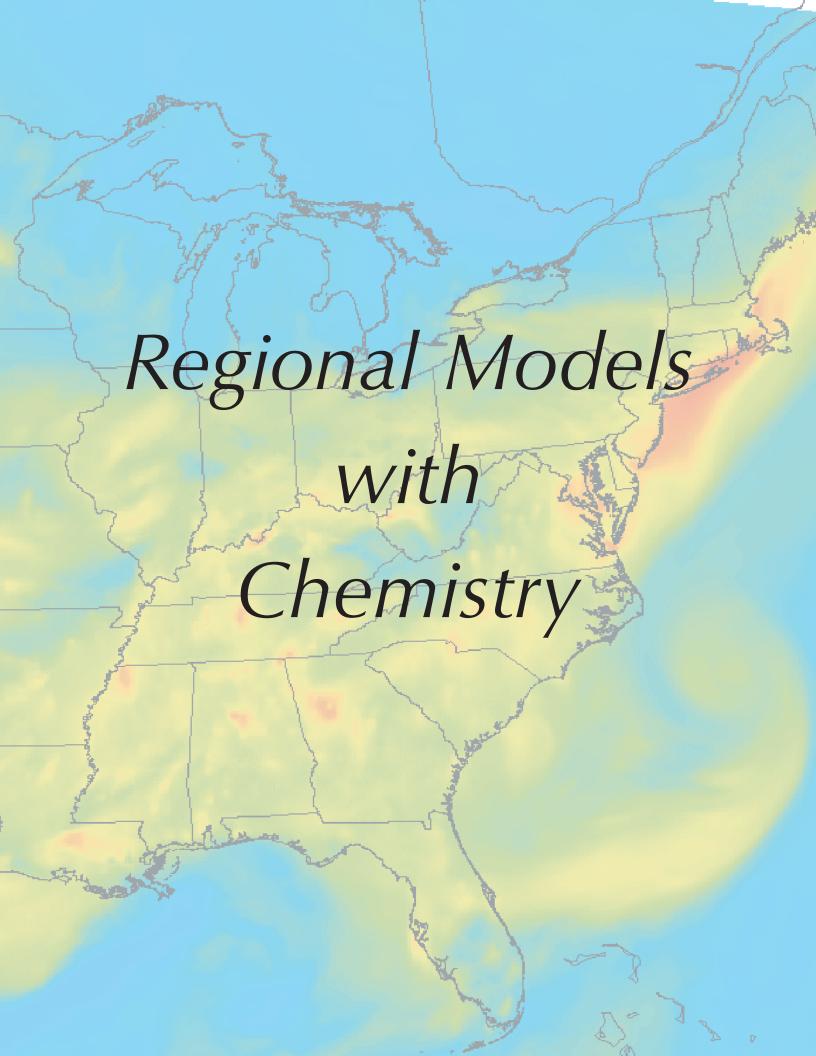
7. Computational requirements

Hardware/software: Linux workstation.

Simulation time: 48-hr trajectory forecast ~20 minutes on Dell Linux workstation.

8. Description of key outcomes, applications (including literature citations describing work), and other information about modeling capabilities

A complete benchmark report discussing the original development, implementation, and evaluation of IDEA is available at the NASA Earth Science Applications Program website http://aiwg.gsfc.nasa.gov/esappdocs/benchmarks/AQI benchmark report v16.doc.



Community Multiscale Air Quality (CMAQ) Modeling System

1. Brief description of model

3-D gridded mesoscale (regional) numerical model for simulation of atmospheric concentrations of tropospheric ozone, particulate matter, acid/nutrient deposition, visibility, air toxics, and mercury.

2. Principal applications or customers

Operational air quality forecast guidance (NOAA/NWS, State agencies, private sector), air quality assessments (EPA, States, Regional Planning Organizations, international community.)

3. Key participants, lab/organization, effort, contact information

Rohit Mathur, ARL/ASMD (rohit.mathur@noaa.gov); Jon Pleim, ARL/ASMD (jonathan.pleim@noaa.gov); Ken Schere, ARL/ASMD (kenneth.schere@noaa.gov).

4. Literature citations, reports, or websites with detailed model description Byun and Schere, *Appl. Mech. Rev.*, 59, 51-77, 2006, www.cmaq-model.org.

5. Specifications

Domain: Urban/regional/continental/inter-continental.

Horizontal resolution and grid/coordinate system: Variable, typically 1-36 km grid cells; nesting capability; generalized coordinate system, typical application: Lambert-conformal map projection with Arakawa-C grid structure.

Vertical resolution and grid/coordinate system: Variable; Example: 34 layers; intervals increase from 38 m near surface to about 1.5 km near domain top of 100 mb (~15.5 km); generalized terrain-following vertical coordinate.

Dynamical and numerical transport schemes: Numerical transport: Piecewise-parabolic method (PPM) positive-definite advection with mass-continuity correction; Dynamics from meteorology driver models (WRF/arw, WRF/nmm, MM5, RAMS, GEM).

Chemistry and aerosol schemes: Gases: CB4, CB05, SAPRC99, in-development: RACM2, SAPRC07; Aerosols: modal model (*Binkowski and Roselle, 2003*), sectional models (MADRID; Univ. of Calif.-Davis).

Planetary boundary layer and land-surface schemes: In meteorology models: Pleim-Xiu (PX) LSM (Pleim and Xiu, 2003, *J. Atmos. Meteo.*, 42, 1811-1822), Asymmetric Convective Model (ACM2, Pleim, 2007a,b, *J. Atmos. Metereol.*); in CMAQ: ACM2 or local eddy-diffusivity.

Deposition schemes: Dry and wet deposition; gases: M3Dry (Byun and Ching, 1999; Pleim et al., *Water, Air, and Soil Pol: Foc, 1,* 243-252, 2001); Aerosols: modally integrated size dependent deposition velocities.

Sub-grid parameterizations: Plume-in grid treatment for major point sources; convective cloud parameterizations (Walcek and Taylor, *J. Atmos. Sci*, *43*, 439-355, 1986), ACM-cloud, Grell cloud now under testing.

6. Sources of required data

Meteorological drivers/boundary conditions: Meteorology drivers (for off-line use of CMAQ): WRF/arw, WRF/nmm; MM5, RAMS, GEM. Analyses for ICs, BCs and FDDA: NCEP/NAM, ECMWF, RUC.

Chemical boundary conditions/assimilations: Static climatological profiles (default or user-defined) or time/space-dependent (from global chemical model, e.g., GEOS-Chem, GFS).

Emission inventories and temporal/spatial processing: Area: EPA NEI 2001/2002; Mobile: Mobile6.0; Biogenics: BEIS3.13; Points: CEMS for major points; Sea-salt: dynamic calculation; Wildfires/blowing dust: under development.

7. Computational requirements

Hardware/software: Unix/Linux cluster (typical example: 8 processors); FORTRAN90; netCDF, IOAPI libraries.

Simulation time: Variable; a 12-km grid simulation (205 grids x 199 grids x 14 grids) of CMAQ on 8 Linux (SGI) processors takes 120 minutes CPU time for a 24-hr simulation.

8. Description of key outcomes, applications (including literature citations describing work), and other information about modeling capabilities

Air quality forecasting:

In a collaborative effort between NOAA/NWS and EPA, CMAQ, driven by WRF/nmm, is used by NCEP for daily opera-

tional forecast guidance for O_3 across the eastern U.S. and experimental O_3 forecast guidance over the continental U.S. A daily developmental PM forecast simulation is also performed over the continental U.S. Model guidance products are publicly available at http://www.weather.gov/aq and have been used by local air quality forecast agencies in developing daily outlooks as well as for in-field guidance during field experiments.

Description of the forecast system: Otte et al., *Weather and Forecasting, 20*, 367-384, 2005. Description of forecast evaluations: Yu et al., *J. Air Waste Mgmt. Assoc., 56*, 1459-1471, 2006; Yu et al., *J. Geophys. Res., in press*, doi:10.1029/2006JD007715, 2007; McKeen et al., *J. Geophys. Res., 112*, D10S20, doi:10.1029/2006JD007608, 2007.

Community modeling applications:

CMAQ is used as an assessment and forecasting model of air quality by a global community of over 500 registered users. The modeling system is peer-reviewed biannually with a publicly-available review report. Model applications are described in proceedings of annual conferences and posted on the CMAS website: http://www.cmascenter.org/conference/archive.cfm. Detailed science model documentation is available at: http://www.epa.gov/asmdnerl/CMAQ/CMAQscienceDoc.html.

Policy/regulatory applications:

The Clean Air Interstate Rule (CAIR, 2005) and the Clean Air Mercury Rule (CAMR, 2005) issued by EPA will bring about significant reductions of NO_x, SO_x, and mercury emissions in the eastern U.S. between now and 2018. The CMAQ model was used in the analyses and regulatory impact assessments during the rulemaking of CAIR and CAMR: http://www.epa.gov/CAIR/pdfs/finaltech02.pdf; http://www.epa.gov/ttn/atw/utility/ria_final.pdf.

States and regions use CMAQ in designing their emission control policies as part of their State Implementation Plans for compliance with air quality standards, e.g., http://pah.cert.ucr.edu/vistas/vistas2/index.shtml.

Diagnostic process studies:

Instrumented versions of CMAQ have been developed to provide process level diagnostics: Process analysis provides detailed information on individual process tendencies and budgets; Sulfur-tracking version provides diagnostic information on modeled sulfate from individual gas- and aqueous pathways; Primary organic carbon aerosol source apportionment.

Weather Research and Forecasting/Chemistry Model (WRF/Chem)

1. Brief description of model

A fully coupled online community model for the prediction and simulation of weather, dispersion, air quality, and regional climate. WRF/Chem may also be run offline for some chemical applications.

2. Principal applications or customers

Air quality, dispersion, weather and regional climate modeling and forecasting, field mission planning and data analysis, impact of emission changes, study of processes that are relevant for global change applications (such as direct and indirect effect of aerosols). There are a large number of national and international users and developers.

- 3. Key participants, lab/organization, effort, contact information Georg Grell, ESRL/GSD, full-time, georg.a.grell@noaa.gov.
- 4. Literature citations, reports, or websites with detailed model description
 Grell et al., Atmos. Environ., 39, 6957-6975, 2005; additional information can be found at http://www.wrf-model.org/WG11/.

5. Specifications

Domain: Hemispheric to local cloud scale. Global version will be available soon.

Horizontal resolution and grid/coordinate system: Variable. Was used by ESRL/PSD down to dx=200m, current real-time application over the contiguous 48 states (20-50°N, 66-130°W), resolution = 27 x 27 km².

Vertical resolution and grid/coordinate system: Terrain following mass vertical coordinate, Arakawa C-grid with different projection options for horizontal coordinates (ARW), rotated lat-lon Arakawa E-Grid for horizontal coordinates of NMM core. Vertical resolution is variable. Example: 34 vertically stretched levels, intervals increase from 40 m near surface to about 1.5 km near domain top of ~20 km.

Dynamical and numerical transport schemes: All available options in two different dynamic cores, the Advanced Research Version (ARW) and the Nonhydrostatic Mesoscale Model (NMM). Mass and scalar conserving, positive definite.

Chemistry and aerosol schemes: Gases: RADM2, CBM-Z, RACM, RACM-MIM, Kinetic PreProcessor (KPP); Aerosols: MADE/SORGAM, MOSAIC.

Planetary Boundary Layer (PBL) and Land-Surface Models (LSM): PBL for hemispheric to mesoscale: Mellor-Yamada-Janjic Turbulent Kinetic Energy (TKE) scheme, Yong-Sei University (YSU) K-profile scheme; PBL for Large Eddy Simulation scales: 3-D TKE closure or Smagorinsky closure. Land-surface: Rapid Update Cycle (RUC), Noah LSM, or simple thermal diffusion.

Deposition schemes: Gases: Wesley (1989), Erisman (1994); Aerosols: Slinn & Slinn (1980), Pleim (1984).

Sub-grid parameterizations: All WRF physics parameterizations.

6. Sources of required data

Meteorological drivers/boundary conditions: Two 3-D-var analysis systems (GSI and WRF-3-D-var) are available to initialize the meteorological variables. Alternatively, any existing model analysis/output may be used if output is in GRIB format. Most commonly used meteorological models are: NCEP-GFS, RUC, NCEP-WRF/NMM, NCEP-Eta, ECMWF-model.

Chemical boundary conditions/assimilations: Boundary conditions from any global Chemical Transport Model (CTM) may be used. Currently used: NCAR-global CTM (MOZART), Mainz Max Planck Institute global CTM, NASA RAQMS model, Japanese global CTM (CHASER). NASA aircraft profiles (McKeen, et al., *J. Geophys. Res.*, doi:10.1029/2001JD000697, 2002).

Emission inventories and temporal/spatial processing: Anthropogenic: EPA NEI 1999 with EPA temporal profiles and 4-km spatial surrogates; Biogenic: BEIS3.11, Guenther [1995]/Simpson [1995].

7. Computational requirements

Hardware/software: Variable. WRF and WRF/Chem will run on many different architectures on single vector processors, OpenMP architectures, and fully distributed memory applications (also mixed OpenMP and distributed) on any number of processors. Most often used are LINUX clusters with 8 - 256 CPUs. FORTRAN90.

Simulation time: Variable, depends on resolution and chemical setup. Dispersion mode is similar cost to meteorology-only run, while chemistry can add a factor of 2 to 20 times the cost of a meteorology-only run (on 1 processor) depending on choice of chemical modules. These numbers will vary even more in the future with new chemistry and aerosol modules becoming available.

However, more sophisticated chemistry usually leads to better scalability on distributed memory parallel computing architectures.

 Description of key outcomes, applications (including literature citations describing work), and other information about modeling capabilities

Model Description:

A fully coupled online community model for the prediction and simulation of weather, dispersion, air quality, and regional climate. WRF/Chem may also be run offline for some chemical applications. It includes two different dynamic cores, the Advanced Research Version (ARW) and the Nonhydrostatic Mesoscale Model (NMM). WRF/Chem is currently used from hemispheric to local cloud-resolving scales. A global version of the ARW core will be available soon. Adjoints of parts of the modeling system are under development. WRF/Chem includes 3-D-var analysis systems for the analysis of meteorological variables (Gridpoint Statistical Interpolation (GSI) and the WRF 3-D-var). Work is underway to include chemical species into the GSI. The development of WRF/Chem is led by scientists from the Earth System Research Laboratory (ESRL).

Outcomes/Applications:

a. Real-time air quality and weather forecasts:

WRF/Chem is used at several institutes to produce simultaneous forecasts of air quality and weather. These include Frontier Research Center in Japan and University of Chile in Santiago de Chile (http://metano.dgf.uchile.cl/cal2.php) during Chilean summer. Starting this summer, it will also be run in real-time to produce ensemble forecasts at the Centro de Previsao de Tempo e Estudos Climaticos (CPTEC) in Brazil. At ESRL, WRF/Chem is used to make twice-daily forecasts of O_3 , PM, their precursors, and meteorological variables over a variety of U.S. domains. Products available at http://www-frd.fsl.noaa.gov/aq/wrf/.

NWS/NCEP is working with GSD to test the impact of in-line and interactive atmospheric-chemistry processes by comparing WRF-NMM-Chem predictions to the NWS operational WRF-CMAQ offline system. WRF-NMM-Chem is a candidate to address NCEP plans to add interactive chemistry effects to its regional and global NWP models.

b. Ensemble ozone and PM_{2.5} forecasting:

WRF/Chem was one of 7 air quality forecast models used to create the first real-time ensemble forecasts for O₃ and PM_{2.5} as part of the 2004 International Consortium for Atmospheric Research on Transport and Transformation/New England Air Quality Study (ICARTT/NEAQS).

McKeen et al., J. Geophys. Res., 110, D21307, doi:10.1029/2005JD005858, 2005.

Pagowski and Grell, J. Geophys. Res., 111, D23S30, doi:10.1029/2006JD007124, 2006.

Pagowski et al., Geophys. Res. Lett., 32, L07814, doi:10.1029/2004GL022305, 2005

Pagowski et al., Atmos. Environ., 40, 3240-3250, 2006.

McKeen et al., J. Geophys. Res., in press, 2007.

c. Mission planning and observational analysis in NOAA field studies:

Real-time WRF/Chem air quality/weather and tracer/weather forecasts were used to help plan observational activities during recent NOAA field missions, including the 2004 ICARTT/NEAQS and the 2006 Texas Air Quality Study (TexAQS). After the missions, observations made on various NOAA platforms were compared with WRF/Chem retrospective calculations. These comparisons contributed to the development of the model components and to the understanding of the emission, chemical evolution, and transport of primary pollutants, O₃, and PM.

Grell et al., Atmos. Environ., 39, 6957-6975, 2005.

McKeen et al., J. Geophys. Res., 110, D21307, doi:10.1029/2005JD005858, 2005.

Frost et al., J. Geophys. Res., 111, D12306, doi:10.1029/2005JD006354, 2006.

McKeen et al., J. Geophys. Res., in press, 2007.

d. Impact of changing NO_x emissions from power generation:

Comparisons of WRF/Chem with NOAA aircraft observations from ICARTT/NEAQS 2004 and with NO_2 column retrievals by the SCIAMACHY and GOME satellites demonstrated that atmospheric NO_x levels have declined in the past decade as a result of the implementation of pollution controls on large fossil-fueled power plants in the eastern U.S. WRF/Chem was used to determine the changes in near-surface O_3 that could be expected in response to these emission declines.

Frost et al., J. Geophys. Res., 111, D12306, doi:10.1029/2005JD006354, 2006.

Kim et al., Geophys. Res. Lett., 33, L22812, doi:10.1029/2006GL027749, 2006.

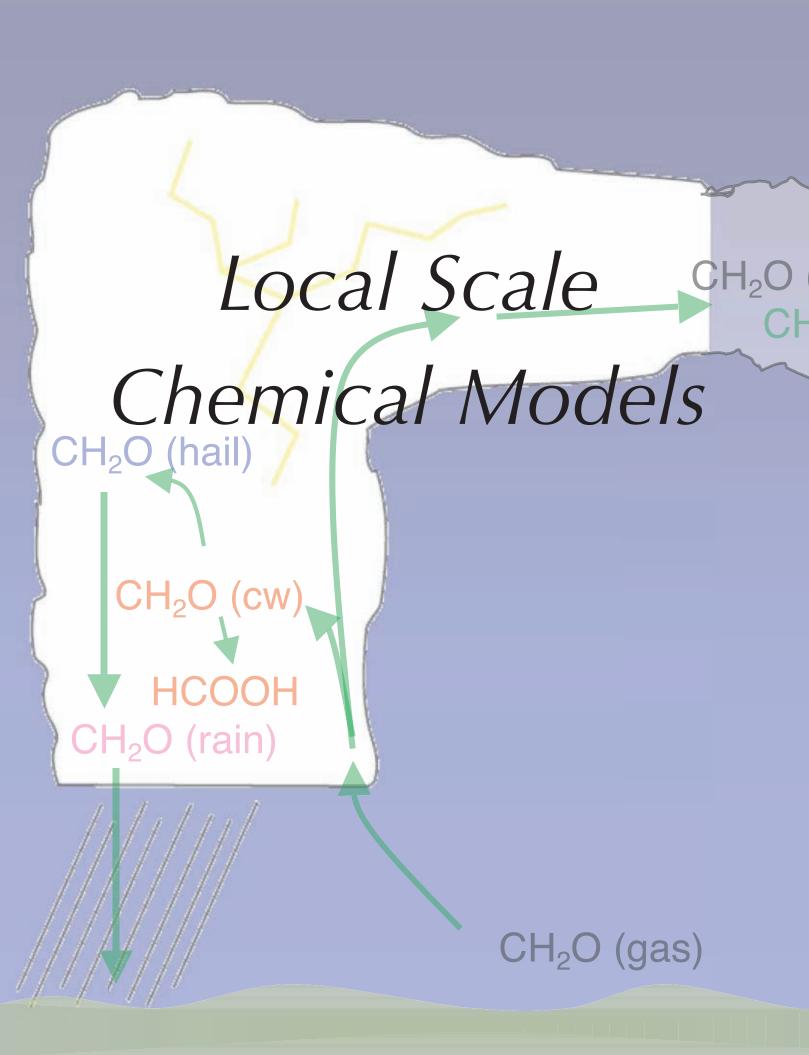
e. Aerosol direct and indirect effect:

Results indicated the importance of the semi-direct and indirect aerosol effect, possibly even for shorter time scales (such as weather forecasting).

Chung et al., J. Geophys. Res., in preparation, 2007.

Fast et al., J. Geophys. Res., 111, D21305, doi:10.1029/2005JD006721, 2006.

Gustafson et al., Geophys. Res. Lett., in review, 2007.



Cloud Parcel

Brief description of model

Adiabatic cloud parcel model including size-resolved microphysics and gas and aqueous phase chemistry. Aerosol/cloud droplets resolved in size categories on a moving grid scale.

Principal applications or customers

Development of cloud microphysics and aqueous phase chemistry schemes.

Key participants, lab/organization, effort, contact information

ESRL/CSD: Barbara Ervens, barbara.ervens@noaa.gov and Graham Feingold, graham.feingold@noaa.gov.

4. Literature citations, reports, or websites with detailed model description

Feingold, G., S.M. Kreidenweis, and Y. Zhang, Stratocumulus processing of gases and cloud condensation nuclei: 1. Trajectory ensemble model, J. Geophys. Res., 103, 19,527-19,542, 1998.

Ervens, B., G. Feingold, G.J. Frost, and S.M. Kreidenweis, A modeling study of aqueous production of dicarboxylic acids: 1. Chemical pathways and organic mass production, J. Geophys. Res., 109, doi: 10.1029/2003JD004387, 2004.

Specifications

Domain: NA

Horizontal resolution and grid/coordinate system: NA Vertical resolution and grid/coordinate system: NA

Dynamical and numerical transport schemes: Lagrangian.

Chemistry and aerosol schemes: Detailed organic gas and aqueous phase chemistry.

Planetary boundary layer and land-surface schemes: NA

Deposition schemes: NA Sub-grid parameterizations: NA

6. Sources of required data

Meteorological drivers/boundary conditions: Adiabatic parcel or kinematic trajectories from host (Eulerian) model.

Chemical boundary conditions/assimilations: NA

Emission inventories and temporal/spatial processing: NA

Computational requirements

Hardware/software: Linux workstation, FORTRAN77.

Simulation time: Minutes to hours.

- Description of key outcomes, applications (including literature citations describing work), and other information about modeling capabilities
 - a. Organic aqueous phase chemistry:

The unique aspect of our model is that it includes an explicit chemistry scheme for organic mass formation in clouds.

Ervens, B., G. Feingold, G.J. Frost, and S.M. Kreidenweis, A modeling study of aqueous production of dicarboxylic acids:

1. Chemical pathways and organic mass production, J. Geophys. Res., 109, doi: 10.1029/2003JD004387, 2004.

Modification of aerosol properties (hygroscopic, CCN) by cloud processing:

Addition of sulfate mass to an initial size distribution affects drop growth rates in subsequent cloud cycles. The version of the model that also includes organic chemistry predicts formation of internally mixed particles with different hygroscopic properties than pure sulfate.

Feingold, G., and S. Kreidenweis, Does cloud processing of aerosol enhance droplet concentrations? J. Geophys. Res, 105, 24,351-24,361, 2000.

Ervens, B., G. Feingold, S.L. Clegg, and S.M. Kreidenweis, A modeling study of aqueous production of dicarboxylic acids: 2. Implications for cloud microphysics, *J. Geophys. Res.*, 109, doi: 10.1029/2004JD004575, 2004.

c. Sensitivity studies to CCN properties:

Studies published to date produce ambiguous results regarding the magnitude and even the sign of the effect of water-soluble organic carbon on cloud drop concentration compared to well-characterized inorganics. We performed theoretical studies for wide ranges of parameters (properties) and concluded that CCN activity of organic aerosols can largely be simplified in cloud models.

Ervens, B., G. Feingold, and S.M. Kreidenweis, The influence of water-soluble organic carbon on cloud drop number concentration, *J. Geophys. Res.*, 110, doi: 10.1029/2004JD005634, 2005.

Regional Atmospheric Modeling System in Large Eddy Simulation mode (RAMS/LES)

1. Brief description of model

A scalable model operated in LES mode with coupled dynamics, size resolved microphysics, and aqueous sulfate chemistry.

2. Principal applications or customers

Analysis of aerosol-cloud interactions and cloud processing of aerosol.

3. Key participants, lab/organization, effort, contact information

Graham Feingold, ESRL/CSD, ~1 FTE, graham.feingold@noaa.gov.

Hongli Jiang, ESRL/CSD, ~ 1FTE, hongli.jiang@noaa.gov..

4. Literature citations, reports, or websites with detailed model description

Feingold, G., and S.M. Kreidenweis, Cloud processing of aerosol as modeled by a large eddy simulation with coupled microphysics and aqueous chemistry, *J. Geophys. Res.*, 107, D23, 4687, doi:10.1029/2002JD002054, 2002, available at www.etl.noaa.gov/~gfeingold.

5. Specifications

Domain: Order 10 km.

Horizontal resolution and grid/coordinate system: Order 100 m.

Vertical resolution and grid/coordinate system: Order 50 m with domain top at \sim 5 km.

Dynamical and numerical transport schemes: RAMS.

Chemistry and aerosol schemes: Aqueous chemistry: sulfate; no gas phase; simple inorganic aerosol (size resolved); absorbing aerosol coupled to radiation.

Planetary boundary layer and land-surface schemes: Explicit convection; Land-surface: LEAF.

Deposition schemes: None over the short simulation periods (few hours).

Sub-grid parameterizations: Deardorff TKE or Smagorinsky type of deformation.

6. Sources of required data

Meteorological drivers/boundary conditions: RAMS model; cyclic BCs for LES (Rawinsonde).

Chemical boundary conditions/assimilations: NA

Emission inventories and temporal/spatial processing: NA

7. Computational requirements

Hardware/software: Single processor linux or iJET (60 CPUs).

Simulation time: Variable. Order days to 1 week.

8. Description of key outcomes, applications (including literature citations describing work), and other information about modeling capabilities

Aerosol-cloud interactions and cloud processing of aerosol.

Approximately 15 publications available at http://www.etl.noaa.gov/~gfeingold.

Master Chemical Mechanism (MCM) - Box Model

1. Brief description of model

A box-model based upon the Leeds Master Chemical Mechanism (MCM).

2. Principal applications or customers

Interpretation and analysis of field campaigns, with focus on gas-phase chemistry.

3. Key participants, lab/organization, effort, contact information

Roberto Sommariva, ESRL/CSD, full-time, Roberto.Sommariva@noaa.gov.

4. Literature citations, reports, or websites with detailed model description

Carslaw et al., J. Geophys. Res., 104, 30,241-30,255, 1999, http://mcm.leeds.ac.uk/MCM.

5. Specifications

Domain: Local/Regional.

Horizontal resolution and grid/coordinate system: NA

Vertical resolution and grid/coordinate system: NA

Dynamical and numerical transport schemes: Zero/One Dimensional.

Chemistry and aerosol schemes: Leeds MCM. For the aerosol scheme, see Sommariva et al., Atmos. Chem. Phys., 6,

1135-1153, 2006.

Planetary boundary layer and land-surface schemes: Estimated from the measurements.

Deposition schemes: See Sommariva et al., Atmos. Chem. Phys., 6, 1135-1153, 2006.

Sub-grid parameterizations: NA

6. Sources of required data

Meteorological drivers/boundary conditions: Mixing height from wind profiler and/or lidar.

Chemical boundary conditions/assimilations: All chemical measurements taken during a field campaign. Essential measurements include: CO, O₃, NO_y, VOCs, photolysis rates.

Emission inventories and temporal/spatial processing: Same as Photochemical Trajectory Model (Derwent et al., *Atmos. Env.*, 32, 2429-2441, 1998), if necessary. Can also use measured emission ratios of key species.

7. Computational requirements

Hardware/software: Windows workstation. FACSIMILE. Could be adapted to work with FORTRAN, KPP, and on a Linux/UNIX workstation (or cluster).

Simulation time: From a few minutes to a few days. Depends on the size of the chemical mechanism, the number of days of the simulation, and the number of constraints of the model.

8. Description of key outcomes, applications (including literature citations describing work), and other information about modeling capabilities

a) Modelling of radicals:

A zero-dimensional box-model fully constrained to measurements of chemical and physical parameters taken on the R/V Brown and on the WP-3D during ICARTT-NEAQS 2004. The model was used to calculate the concentrations of radicals (OH, HO₂, RO₂, NO₃) to compare with the measurements made during the campaign.

Osthoff et al., J. Geophys. Res., 111, D23, doi:10.1029/2006JD007593, 2006.

Sommariva et al., Modelling studies of radicals in the marine boundary layer during NEAQS-ITCT 2004, in preparation.

b) Simulation of urban plumes:

Box-model initialized with emission ratios determined during NEAQS 2002 and 2004 campaigns to simulate the gas-phase evolution of a typical urban plume. The model was used to study the formation of HNO₃, alkyl nitrates, oxygenated VOCs, PANs and ClNO₂.

Neuman et al., J. Geophys. Res., 111, D23, doi:10.1029/2005JD007010, 2006.

Roberts et al., Measurements of PANs during the New England Air Quality Study 2002, *J. Geophys. Res.*, submitted. Osthoff et al., Observation of ClNO₂, a significant chlorine atom source in the marine boundary layer, submitted.

Sommariva et al., A study of secondary organic chemistry in an urban plume with a Master Chemical Mechanism, in preparation.

c. Additional Information:

The model is essentially an application of the Leeds MCM. Therefore it can be easily adapted to other applications and extended. Possible uses are: coupling with a multiphase chemical mechanism, more detailed treatment of the gas-aerosol interface, addition of SOA formation mechanism, adaptation of the Photochemical Trajectory Model to U.S. conditions, etc.

Model of Aerosols and Ions in the Atmosphere (MAIA)

1. Brief description of model

MAIA solves the differential equations describing a system of neutral and negative sulfate aerosol particles. A particular strength of the model is its ability to resolve the formation of small sulfuric acid/water clusters from the gas phase as well as their growth to larger (CCN) sizes. Small sulfuric acid/water clusters are described with a molecular size resolution, larger aerosol particles with geometric size sections. A first order scheme resolving the aerosol size distribution within these sections efficiently suppresses numerical diffusion. Laboratory thermodynamic data for sulfuric acid uptake and loss by small neutral and charged clusters are used, allowing for a reliable description of both neutral and charged nucleation down to the very low temperatures occurring in the upper troposphere and lower stratosphere. Different versions of the model exist, including a global box model version, and a Lagrangian version, which can be run on trajectories inside and outside of clouds.

2. Principal applications or customers

Aerosol modeling.

3. Key participants, lab/organization, effort, contact information

Jan Kazil (University of Colorado/CIRES), Edward R. Lovejoy (NOAA).

4. Literature citations, reports, or websites with detailed model description

Kazil, J., E.R. Lovejoy, E.J. Jensen, and D.R. Hanson, Is aerosol formation in cirrus clouds possible? *Atmos. Chem. Phys.*, 7, 1407-1413, 2007.

Kazil, J., E.R. Lovejoy, M.C. Barth, and K. O'Brien, Aerosol nucleation over oceans and the role of galactic cosmic rays, *Atmos. Chem. Phys.*, 6, 4905–4924, 2006.

Lovejoy, E.R., J. Curtius, and K.D. Froyd, Atmospheric ion-induced nucleation of sulfuric acid and water, *J. Geophys. Res.*, 109, D08204, doi:10.1029/2003JD004460, 2004.

5. Specifications

Domain: Box model, Lagrangian model.

Horizontal resolution and grid/coordinate system: Variable/Lagrangian.

Vertical resolution and grid/coordinate system: Variable/Lagrangian.

Dynamical and numerical transport schemes: Variable/Lagrangian.

Chemistry and aerosol schemes: Steady state OH photochemistry, neutral and ion-induced sulfate aerosol nucleation, sulfate aerosol growth by condensation and coagulation, sulfate aerosol loss onto other types of aerosol and onto cloud droplets and ice crystals.

Planetary boundary layer and land-surface schemes: None.

Deposition schemes: None.

Sub-grid parameterizations: None.

6. Sources of required data

Meteorological drivers/boundary conditions: Global chemistry and transport models, Large Eddy Simulations, 2-D cirrus cloud models.

Chemical boundary conditions/assimilations: None.

Emission inventories and temporal/spatial processing: None.

7. Computational requirements

Hardware/software: Contemporary Personal Computer; Linux/UNIX OS, GNU Make, netCDF library, Intel FORTRAN77 compiler. Simulation time: Minutes for box and Lagrangian simulations, days for global box model simulations.

 Description of key outcomes, applications (including literature citations describing work), and other information about modeling capabilities

Kazil, J., E.R. Lovejoy, E.J. Jensen, and D.R. Hanson, Is aerosol formation in cirrus clouds possible? *Atmos. Chem. Phys.*, 7, 1407-1413, 2007.

Abstract. The recent observation of ultrafine aerosol particles in cirrus clouds has raised the question whether aerosol formation within cirrus clouds is possible, and if so, what mechanisms are involved. We have developed an aerosol parcel model of neutral and charged H₂SO₄/H₂O aerosol processes, including nucleation from the gas phase and loss onto cirrus ice particles. Laboratory thermodynamic data for sulfuric acid uptake and loss by small neutral and charged clusters are used, allowing for a reliable description of both neutral and charged nucleation down to the very low temperatures occurring in the upper troposphere and lower stratosphere. The model implements a first order scheme for resolving the aerosol size distribution within its geometric size sections, which efficiently suppresses numerical diffusion. We operate the model offline on trajectories generated with a detailed 1-D cirrus model which describes ice crystal nucleation, deposition growth, vertical advection of ice crystals and water vapor, and ice crystal sedimentation. In this paper we explore the possibility of aerosol formation within non-convective cirrus clouds and draw conclusions for aerosol formation in anvil cirrus. We find that sulfate aerosol formation within cirrus clouds can proceed even at high ice surface area concentrations, and depends strongly on the size of the cirrus ice crystals and on the surface area concentration of preexisting aerosol particles.

Kazil, J., E.R. Lovejoy, M.C. Barth, and K. O'Brien, Aerosol nucleation over oceans and the role of galactic cosmic rays, *Atmos. Chem. Phys.*, *6*, 4905–4924, 2006.

Abstract. We investigate formation of sulfate aerosol in the marine troposphere from neutral and charged nucleation of H₂SO₄ and H₂O. A box model of neutral and charged aerosol processes is run on a grid covering the oceans. Input data are taken from a model of galactic cosmic rays in the atmosphere, and from global chemistry and transport models. We find a weak aerosol production over the tropical oceans in the lower and middle troposphere, and a stronger production at higher latitudes, most notably downwind of industrial regions. The strongest aerosol production however occurs in the upper troposphere over areas with frequent convective activity, in particular in the tropics. This finding supports the proposition by which non-sea salt marine boundary layer aerosol in tropical regions does not form in situ, but nucleates in the upper troposphere from convectively lifted and cloud processed boundary layer air rich in aerosol precursor gases, from where it descends in subsiding air masses compensating convection. Convection of boundary layer air also appears to drive the formation of condensation nuclei in the tropical upper troposphere which maintains the stratospheric aerosol layer in the absence of volcanic activity. Neutral nucleation contributes only marginally to aerosol production in our simulations. This highlights the importance of other mechanisms, including charged binary and ternary, and neutral ternary nucleation for aerosol formation. Our analysis indicates that the variation of ionization by galactic cosmic rays over the decadal solar cycle does not entail a response in aerosol production and cloud cover via the second indirect aerosol effect that would explain observed variations in global cloud cover. We estimate that the variation in radiative forcing resulting from a response of clouds to the change in galactic cosmic ray ionization and subsequent aerosol production over the decadal solar cycle is smaller than the concurrent variation of total solar irradiance.

Lovejoy, E.R., J. Curtius, and K.D. Froyd, Atmospheric ion-induced nucleation of sulfuric acid and water, *J. Geophys. Res.*, 109, D08204, doi:10.1029/2003JD004460, 2004.

Abstract. Field studies show that gas phase nucleation is an important source of new particles in the Earth's atmosphere. However, the mechanism of new particle formation is not known. The predictions of current atmospheric nucleation models are highly uncertain because the models are based on estimates for the thermodynamics of cluster growth. We have measured the thermodynamics for the growth and evaporation of small cluster ions containing H_2SO_4 and H_2O , and incorporated these data into a kinetic aerosol model to yield quantitative predictions of the rate of ion-induced nucleation for atmospheric conditions. The model predicts that the binary negative ion H_2SO_4/H_2O mechanism is an efficient source of new particles in the middle and upper troposphere. The ion-induced $HSO_4^-/H_2SO_4/H_2O$ mechanism does explain nucleation events observed in the remote middle troposphere, but does not generally predict the nucleation events observed in the boundary layer.



NOAA Atmospheric Chemical Modeling Contact List

First Name	Last Name	Affiliation	Email
Arlyn	Andrews Angevine Austin Bao Benjamin	ESRL/GMD	arlyn.andrews@noaa.gov
Wayne		ESRL/CSD	wayne.m.angevine@noaa.gov
John		GFDL	john.austin@noaa.gov
Jian-wen		ESRL/PSD	jian-wen.bao@noaa.gov
Stan		ESRL/GSD	stan.benjamin@noaa.gov
Prakash Rainer Jerome John Lori	Brave Bleck Brioude Brown Bruhwiler	ARL ESRL/GSD ESRL/CSD ESRL/GSD ESRL/GMD	prakash.bhave@noaa.gov rainer.bleck@noaa.gov jerome.brioude@noaa.gov john.m.brown@noaa.gov lori.bruhwiler@noaa.gov
Jim	Butler	ESRL/GMD	james.h.butler@noaa.gov
Mark	Cohen	ARL	mark.cohen@noaa.gov
Owen	Cooper	ESRL/CSD	owen.r.cooper@noaa.gov
John	Daniel	ESRL/CSD	john.s.daniel@noaa.gov
Paula	Davidson	NWS/OST	paula.davidson@noaa.gov
Thomas	Delworth	GFDL	tom.delworth@noaa.gov
Roland	Draxler	ARL	roland.draxler@noaa.gov
Christine	Ennis	ESRL/CSD	christine.a.ennis@noaa.gov
Barbara	Ervens	ESRL/CSD	barbara.ervens@noaa.gov
Songmiao	Fan	GFDL	songmiao.fan@noaa.gov
Graham	Feingold	ESRL/CSD	graham.feingold@noaa.gov
Steven	Fine	ARL	steven.fine@noaa.gov
Arlene	Fiore	GFDL	arlene.fiore@noaa.gov
Debe	Dailey-Fisher	ESRL/CSD	d.a.fisher@noaa.gov
Greg	Frost	ESRL/CSD	gregory.j.frost@noaa.gov
Alice	Gilliland	ARL GFDL ESRL/CSD ESRL/GSD ESRL/GMD	alice.gilliland@noaa.gov
Paul	Ginoux		paul.ginoux@noaa.gov
Claire	Granier		claire.granier@noaa.gov
Georg	Grell		georg.a.grell@noaa.gov
Adam	Hirsch		adam.hirsch@noaa.gov
David	Hofmann	ESRL/GMD	david.j.hofmann@noaa.gov
Larry	Horowitz	GFDL	larry.horowitz@noaa.gov
Ho-Chun	Huang	NWS/NCEP	ho-chun.huang@noaa.gov
Janet	Intrieri	ESRL/CSD	janet.intrieri@noaa.gov
Mark	Iredell	NWS/NCEP	mark.iredell@noaa.gov
Andy	Jacobson	ESRL/GMD	andy.jacobson@noaa.gov
Hongli	Jiang	ESRL/CSD	hongli.jiang@noaa.gov
Jan	Kazil	ESRL/CSD	jan.kazil@noaa.gov
Ann	Keane	ESRL	ann.keane@noaa.gov
Barb	Keppler	ESRL/CSD	barbara.a.keppler@noaa.gov
Si-Wan	Kim	ESRL/CSD	siwan.kim@noaa.gov
Steven	Koch	ESRL/GSD	steven.koch@noaa.gov
Shobha	Kondragunta	NESDIS/STAR	shobha.kondragunta@noaa.go
Rhonda	Lange	ESRL	rhonda.k.lange@noaa.gov
Jin	Lee	ESRL/GSD	jin.lee@noaa.gov
Chip (Hiram)	Levy	GFDL	hiram.levy@noaa.gov
Stephen	Lord	NWS/NCEP	stephen.lord@noaa.gov
Edward	Lovejoy	ESRL/CSD	edward.r.lovejoy@noaa.gov
Sarah	Lu	NWS/NCEP	sarah.lu@noaa.gov
Alexander	MacDonald	ESRL	alexander.e.macdonald@noaa

Contact List, continued

First Name	Last Name	Affiliation	Email
Melinda	Marquis	ESRL	melinda.marquis@noaa.gov
Rohit	Mathur	ARL	rohit.mathur@noaa.gov
Stuart	McKeen	ESRL/CSD	stuart.a.mckeen@noaa.gov
Jeff	McQueen	NWS/NCEP	jeff.mcqueen@noaa.gov
Jim	Meagher	ESRL/CSD	james.f.meagher@noaa.gov
Jacques	Middlecoff	ESRL/GSD	jacques.middlecoff@noaa.go
John	Miller	ESRL/GMD	john.b.miller@noaa.gov
Yi	Ming	GFDL	yi.ming@noaa.gov
Shrinivas	Moorthi	NWS/NCEP	shrinivas.moorthi@noaa.gov
Bud (Walter)	Moxim	GFDL	bud.moxim@noaa.gov
Sreela	Nandi	NWS/OST	sreela.nandi@noaa.gov
William	Neff	ESRL/PSD	william.nett@noaa.gov
Mariusz	Pagowski	ESRL/GSD	mariusz.pagowski@noaa.gov
Steven	Peckham	ESRL/GSD	steven.peckham@noaa.gov
Wouter	Peters	ESRL/GMD	wouter.peters@noaa.gov
Gabrielle	Petron	ESRL/GMD	gabrielle.petron@noaa.gov
Brad	Pierce	NESDIS/STAR	brad.pierce@noaa.gov
Rob	Pinder	ARL	rob.pinder@noaa.gov
Jon	Pleim	ARL	pleim.jon@epamail.epa.gov
Robert	Portmann	ESRL/CSD	robert.w.portmann@noaa.gov
V. (Ram)	Ramaswamy	GFDL	v.ramaswamy@noaa.gov
A.R. (Ravi)	Ravishankara	ESRL/CSD	a.r.ravishankara@noaa.gov
Karen	Rosenlof	ESRL/CSD	karen.h.rosenlof@noaa.gov
Ken	Schere	ARL	kenneth.schere@noaa.gov
Susan	Solomon	ESRL/CSD	susan.solomon@noaa.gov
Roberto	Sommariva	ESRL/CSD	roberto.sommariva@noaa.go
Ariel	Stein	ARL	ariel.stein@noaa.gov
Pieter	Tans	ESRL/GMD	pieter.tans@noaa.gov
Fred	Toepfer	NWS/NCEP	frederick.toepfer@noaa.gov
Michael	Trainer	ESRL/CSD	michael.k.trainer@noaa.gov
Louis W.	Uccellini	NWS/NCEP	louis.uccellini@noaa.gov
Jeanne	Waters	ESRL/CSD	jeanne.s.waters@noaa.gov
Jim	Wilczak	ESRL/PSD	james.m.wilczak@noaa.gov
John	Wilson	GFDL	john.wilson@noaa.gov